

Reaction Operations

Reaction (Batch Stoichiometric)

This operation is used to represent any number of material transformations that take place in a stirred tank operating in batch mode and for which kinetic expressions are unknown or unimportant. It is possible to have simultaneous feeding of reactants during the reaction, if the Fed Batch options are selected/specified

Material Balances

The reactions are assumed to occur in a sequence (one after the other). In that sense, the calculations assume that the product mixture of the first reaction is the reacting mixture of the second, and so on.

The user provides the mass or molar stoichiometric coefficients (A_i) of the various components for each reaction and the extent of reaction (x) based on either the limiting component or a reference component. Negative stoichiometric coefficients are used for reactants and positive for products. The coefficients can be supplied in either mass or molar units. The algorithm used by the program to perform the material balances for each reaction is explained in the following paragraphs.

If the extent of the reaction is expressed based on the limiting component then, first of all, the limiting component is identified. This is done based on the mass stoichiometry and the composition of the reacting mixture. If the extent of the reaction is expressed based on a user-defined component, then first of all, the program attempts to validate that the user-defined conversion is achievable (i.e., there are enough reactants for the reaction to proceed to such an extent). If that is not the case, then the conversion (x) is adjusted to reflect the maximum achievable conversion percentage (based on the extent-component chosen by the user).

For the limiting component (k) or the extent-reference component (depending on what is the case) the following holds:

$$F_{out_k} = F_{in_k}(1 - x),$$

where,

F_{out_k} is the mass flowrate of the component after the reaction,

F_{in_k} is the mass flowrate of the component before the reaction, and

x is the (possibly adjusted) reaction extent.

Now, the mass flowrate after the reaction (F_{out_i}) of any other component present (i) as a function of its mass flowrate (F_{in_i}) before the reaction, the extent of reaction (x), and the mass stoichiometric coefficients (A_i), is given by the following equation:

$$F_{out_i} = F_{in_i} - F_{in_k} x \left(\frac{A_i}{A_k} \right),$$

where A_k is the coefficient of the limiting or extent-reference component.

The same algorithm is repeated for all reactions specified using the product-mixture of reaction N-1 as the feed of reaction N.

Emissions

You may also specify (through the Emissions tab) the percentage of each component (at the end of all reactions) that ends up in the gas exhaust stream.

Reaction Temperature and Heating/Cooling Requirements

To estimate the overall heating or cooling requirements, the model considers:

- ◆ the enthalpy of each reacting mixture
- ◆ the temperature of each reaction
- ◆ the heat released or absorbed by each reaction as calculated based on the reaction extent and a user-defined enthalpy-reference component

The temperature of the last reaction determines the exit temperature of the process step which is displayed on the Operating Conditions tab. The heating and cooling requirements are summed up over all the reactions taking place, and the total is reported as the total heating (in kcal/h) and total cooling (in kcal/h) on the Oper. Conditions tab. Furthermore, based on your choices for heat transfer agents for each reaction, the demands for each agent are calculated and reported in the economic evaluation report.

Power Consumption

The average agitation power is estimated by multiplying the agitation rate (kW/m³ of liquid mixture) by the total liquid volume of the step. It is assumed that all agitation power eventually dissipates into heat that contributes to the heating or cooling requirements of the step.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the

Operation Mode dialog of the procedure. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

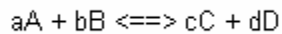
In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Reaction (Batch Equilibrium)

This operation can handle any number of equilibrium reactions and supports a wide variety of reaction equilibrium expressions. It computes the conversion for any number of simultaneous reactions based on the equilibrium constants, the stoichiometric coefficients, and the component concentration exponents that the user specifies.

Material Balances

Consider the following equilibrium reaction



Define the extent of reaction, ξ , as follows:

$$d\xi = -dn_A/a = -dn_B/b = dn_C/c = dn_D/d$$

If ν_i is the stoichiometric coefficient of component i (negative for reactants, positive for products), the above equation can be rewritten as

$$dn_i = \nu_i d\xi$$

and for multiple reactions, the above equation becomes

where q is the number of simultaneous reactions, n_{i0} is the mole flowrate of component i in the feed, and n_i is the mole flowrate of component i in the outlet stream (at equilibrium). Further, for each reaction j we have the equilibrium relationship which can be written as:

$$K_{eq_j} - \left[\prod_{i=1}^N (C_i)^{\alpha_{ij}} \right]_j = 0.0 \quad \text{for } j=1, \dots, q$$

If $\xi = [\xi_1, \xi_2, \dots, \xi_q]$ is used as a vector of independent variables with an initial value of zero, the above equations become equivalent to a system of nonlinear algebraic equations which are solved numerically for ξ . Substitution of the calculated ξ values into the above equations yields the composition of the reaction mixture at equilibrium. For the non-isothermal case, the temperature of the mixture T is another unknown and the energy balance relationship provides the additional equation for solving the system.

To account for emissions, the user can specify the percentage of each component that is emitted. Please note that the specified percentage is based on the composition of the reaction mixture after equilibrium is reached.

Thermal Mode

The equilibrium reactor can operate isothermally, adiabatically or with a specified heating or cooling duty. For adiabatic operation or for specified heating or cooling duty, the equilibrium temperature is an unknown variable that is calculated by the model. For isothermal operation (specified operating temperature), the energy balance equation is used to calculate the heating or cooling requirement.

Power Consumption

The average agitation power is estimated by multiplying the agitation rate (kW/m^3 of liquid mixture) by the total liquid volume of the step. It is assumed that all agitation power eventually dissipates into heat that contributes to the heating or cooling requirements of the step.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of

material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

References

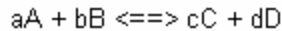
Fogler, H. S. 1992. Elements of Chemical Reaction Engineering, 2nd edition, Prentice Hall.

Reaction (Continuous Equilibrium)

This operation can handle any number of equilibrium reactions and supports a wide variety of reaction equilibrium expressions. It computes the conversion for any number of simultaneous reactions based on the equilibrium constants, the stoichiometric coefficients, and the component concentration exponents that the user specifies.

Material Balances

Consider the following equilibrium reaction



Define the extent of reaction, ξ , as follows:

$$d\xi = -dn_A/a = -dn_B/b = dn_C/c = dn_D/d$$

If ν_i is the stoichiometric coefficient of component i (negative for reactants, positive for products), the above equation can be rewritten as

$$dn_i = \nu_i d\xi$$

and for multiple reactions, the above equation becomes

$$dn_i = \sum_{j=1}^q \nu_{ij} d\xi_j \quad \text{or} \quad n_i = n_{i0} + \sum_{j=1}^q \nu_{ij} \xi_j$$

where q is the number of simultaneous reactions, n_{i0} is the mole flowrate of component i in the feed, and n_i is the mole flowrate of component i in the outlet stream (at equilibrium). Further, for each reaction j we have the equilibrium relationship which can be written as:

$$K_{eqj} - \left[\prod_{i=1}^N (C_i)^{\alpha_i} \right]_j = 0.0 \quad \text{for } j=1, \dots, q$$

If $\xi = [\xi_1, \xi_2, \dots, \xi_q]$ is used as a vector of independent variables with an initial value of zero, the above equations become equivalent to a system of nonlinear algebraic equations which are solved numerically for ξ . Substitution of the calculated ξ values into the above equations yields

the composition of the reaction mixture at equilibrium. For the non-isothermal case, the temperature of the mixture T is another unknown and the energy balance relationship provides the additional equation for solving the system.

To account for emissions, the user can specify the percentage of each component that is emitted. Please note that the specified percentage is based on the composition of the reaction mixture after equilibrium is reached.

Thermal Mode

The equilibrium reactor can operate isothermally, adiabatically or with a specified heating or cooling duty. For adiabatic operation or for specified heating or cooling duty, the equilibrium temperature is an unknown variable that is calculated by the model. For isothermal operation (specified operating temperature), the energy balance equation is used to calculate the heating or cooling requirement.

Power Consumption

The average agitation power is estimated by multiplying the agitation rate (kW/m^3 of liquid mixture) by the total liquid volume of the step. It is assumed that all agitation power eventually dissipates into heat that contributes to the heating or cooling requirements of the step.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

References

Fogler, H. S. 1992. Elements of Chemical Reaction Engineering, 2nd edition, Prentice Hall.

Reaction (Batch Kinetic)

This operation can be used to model any number of parallel or sequential reactions (material transformations) that take place in a batch, stirred tank reactor. It supports a wide variety of reaction kinetics. A reaction can be initiated at a specific time relative to the beginning of the step's process time or when the concentration of a certain component exceeds or drops below a certain value. Similarly, a reaction can be terminated at a specific time relative to the end of the step's process time or when the concentration of a certain component exceeds or drops below a certain value. The contents of the reaction mixture are assumed well mixed at any time point. It is possible to have simultaneous feeding of reactants during the reaction, if the Fed Batch options are selected/ specified.

Material Balances

For a component A that reacts in a batch reactor, the generalized component balance is given by the following equation:

$$\frac{dN_A}{dt} = r_A \cdot V + F_0 \cdot x_A$$

where V is volume of material in the reactor, N_A is the amount (mass/moles) of component A, r_A is the combined reaction rate of component A as a function of time, F_0 is the (mass/ molar) flowrate of the feed stream (in the case of simultaneous feeding) and x_A is the (mass /mole) fraction of component A in the feed stream. (If the amount of components is expressed in terms of mass, then F_0 is a mass flow rate and x_A is the mass fraction of component A and if the amount is in moles then F_0 is a molar flow rate and x_A is the mole fraction.)

The (mass / molar) concentration of a component A is given by:

$$C_A = \frac{N_A}{V}$$

In the case of no feed stream (fed batch options are not selected) and constant density system the component balance reduces to:

$$dC_A = r_A \cdot dt$$

The component A reaction rate r_A is given by:

$$r_A = \sum_{j=1}^q r_{Aj}$$

where r_{Aj} is the reaction rate of component A due to reaction j and q is the total number of reactions. If K is the rate reference component of reaction j, then, the reaction rate of component A due to reaction j is given by the following equation:

$$r_{Aj} = \frac{v_{Aj}}{v_{kj}} (r_{kj})$$

where v_{Aj} and v_{kj} are the stoichiometric coefficients of components A and K in reaction j and can be specified on mass or molar basis. Negative stoichiometric coefficients are used for reactants

and positive for products. The general rate expression (based on the rate reference component) of a reaction j is given by the following equation:

$$r_j = \frac{k \prod_{i=1}^N (C_i)^{\alpha_i}}{K1 + C_m + C_n / K2}$$

where C_i [kmol/m³] is the concentration of component i [kmol/m³] and α_i is the order of the j th reaction with respect to component i . $K1$ and $K2$ are user-specified constants. C_m [kmol/m³] and C_n [kmol/m³] are the concentrations of components m and n that are identified by the user. N is the total number of reactions. The reaction rate constant k is either specified by the user or calculated using an Arrhenius expression:

$$k_j = A_j \exp\left(-\frac{E_j}{RT}\right)$$

where A_j is the pre-exponential factor (or frequency factor) and E_j is the activation energy of the j th reaction. **Please be careful when you select the units and specify the values of k_j or A_j .** The units of the overall rate expression must be in kmol/m³-s.

The above equations written for each component reacting in a batch reactor constitute a system of ordinary differential equations that are integrated numerically to calculate the final composition of the reacting mixture. The integration time is equal to the process time of the unit. A reaction, however, can be initiated or terminated at any time during that time period using the 'Start' and 'End' reaction criteria.

For systems of variable reaction mixture density (which is often the case for gaseous reactions), the simplified overall material balance equation cannot be used. An excellent description of the formulation used in that case can be found in the literature (Fogler, 1992 - pp. 505-510).

The model performs rigorous VOC emission calculations for any of the following cases: 1) The reaction takes place under gas sweep conditions; 2) A gaseous component is released during the reaction that results in VOC emissions; and 3) The reaction takes place under vacuum and the leakage of air results in emissions.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Thermal Mode

A batch reactor can operate isothermally (at a constant operating temperature), adiabatically (no exchange of heat with the surroundings), or with an evenly distributed heating or cooling

duty during the process time. Under isothermal conditions, the model calculates the heating or cooling requirement as a function of time. Read the "Profiles" paragraph for information on how to view and plot the heating and cooling requirement as a function of time. The heating/cooling duty displayed on the first dialog window in kcal/h represents averaged values over the process time of the unit. Under conditions of specified heating or cooling duty of constant rate, the model calculates the temperature of the reacting mixture as a function of time (see "Profiles" below for information on how to view or plot the temperature profiles). Adiabatic operation is a special case of specified heating or cooling duty.

Power Consumption

The average agitation power is estimated by multiplying the agitation rate (kW/m^3 of liquid mixture) by the total liquid volume of the step. It is assumed that all agitation power eventually dissipates into heat that contributes to the heating or cooling requirements of the operation.

References

Fogler, H. S. 1992. Elements of Chemical Reaction Engineering, 2nd edition, Prentice Hall.

Reaction (Continuous Kinetic)

This operation can be used to model any number of parallel or sequential reactions (material transformations) that take place continuously in a stirred tank reactor. It supports a wide variety of reaction kinetics. The inlet streams are assumed to be perfectly (and instantaneously) mixed with the material already in the reactor, so that the outlet stream composition is identical to that of the reactor contents.

Material Balances

For a component A that enters this process step, the mass balance equation for a constant density system is given by the following equation:

$$0 = F C_{in} - F C - V_w r_A$$

where F is the volumetric flowrate, C_{in} is the inlet concentration of component A, C is the outlet concentration of component A, and r_A is the combined reaction rate of component A, given by:

$$r_A = \sum_{j=1}^q r_{Aj}$$

where r_{Aj} is the reaction rate of component A due to reaction j and q is the overall number of reactions. If k is the rate reference component of reaction j , then, the reaction rate of component A due to reaction j is given by the following equation:

$$r_{Aj} = \frac{v_{Aj}}{v_{kj}} (r_{kj})$$

where v_{Aj} and v_{kj} are the stoichiometric coefficients of components A and k in reaction j and can be specified on a mass or molar basis. Negative stoichiometric coefficients are used for reactants and positive for products. The general rate expression (based on the rate reference component) of a reaction j is given by the following equation:

$$r_j = \frac{k \prod_{i=1}^N (C_i)^{\alpha_i}}{K1 + Cm + Cn / K2}$$

where C_i [kmol/m³] is the concentration of component i and α_i is the order of the j th reaction with respect to component i . $K1$ and $K2$ are user-specified constants. Cm [kmol/m³] and Cn [kmol/m³] are the concentrations of components m and n that are identified by the user. N is the total number of reactions. The reaction rate constant k is either specified by the user or calculated using an Arrhenius expression:

$$k_j = A_j \exp\left(-\frac{E_j}{RT}\right)$$

where A_j is the pre-exponential factor (or frequency factor) and E_j is the activation energy of the j th reaction. **Please be careful when you select the units and specify the values of k_j or A_j .** The units of the overall rate expression must be in kmol/m³-s.

The above equations written for each component entering this unit constitute a set of non-linear equations which is solved numerically to calculate the outlet stream concentration.

For systems of variable reaction mixture density (which is often the case for gaseous reactions), the simplified overall material balance equation cannot be used. An excellent description of the formulation used in that case can be found in the literature (Fogler, 1992 - pp. 505-507).

To account for emissions, the user can specify the percentage of each component that is emitted. Please note that the specified percentage is based on the composition of the outlet stream (after the completion of the reaction).

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Thermal Mode

Three thermal modes of operation are available: Isothermal, Adiabatic, Set Heating or Cooling Duty. In the isothermal case, the system calculates the required heating or cooling duty. In the other two cases, it calculates the operating temperature.

Power Consumption

The average agitation power is estimated by multiplying the agitation rate (kW/m^3 of liquid mixture) by the total liquid volume of the step. It is assumed that all agitation power eventually dissipates into heat that contributes to the heating or cooling requirements of the step.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

References

Fogler, H. S. 1992. Elements of Chemical Reaction Engineering, 2nd edition, Prentice Hall.

PF-Reaction (Continuous Stoichiometric)

This operation is used to represent material transformations that take place in a plug-flow reactor for which kinetic expressions are unknown or unimportant.

Material Balances

The user provides the mass stoichiometric coefficients (A_i) of the various components and the extent of reaction (x) based on the limiting component. Negative stoichiometric coefficients are used for reactants and positive for products.

The limiting component is identified based on the mass stoichiometry and the composition of the reacting mixture. For the limiting component (k) the following holds:

$$F_{out_k} = F_{in_k} (1 - x),$$

where,

F_{out_k} is the mass flowrate of the component after the reaction,

F_{in_k} is the mass flowrate of the component before the reaction, and

x is the (possibly adjusted) reaction extent.

Now, the mass flowrate after the reaction (F_{out_i}) of any other component present (i) as a function of its mass flowrate (F_{in_i}) before the reaction, the extent of reaction (x), and the mass stoichiometric coefficients (A_i), is given by the following equation:

$$F_{out_i} = F_{in_i} - F_{in_k} x \left(\frac{A_i}{A_k} \right),$$

where A_k is the coefficient of the limiting or extent-reference component.

Heating/Cooling Requirement

To estimate the overall heating or cooling requirement, the model considers:

- ◆ the enthalpy of the reacting mixture
- ◆ the operating (exit) temperature
- ◆ the heat released or absorbed by the reaction as calculated based on the reaction extent and a user-defined enthalpy-reference component

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical

units operating in parallel with a total vessel volume equal to the calculated. The working to vessel volume ratio has a default value of 100%. Presence of catalyst or other packing material may result in working to vessel volume ratios of less than 100%.

In Rating Mode, the user specifies the vessel volume, the number of units, and the working to vessel volume ratio and the system calculates the residence time.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

PF-Reaction (Continuous Kinetic)

This operation can model any number of parallel or sequential reactions that take place in a Plug Flow Reactor (PFR). It supports a wide variety of reaction kinetics. The model assumes that the flow in the tube is radially isotropic (without mass or energy gradients) and that axial mixing is negligible.

Vessel Size Estimation

In design mode of calculation, the user provides the reactor **Space Time** (the ratio of the working vessel volume to the actual volumetric flowrate of the inlet stream) and the model calculates the working vessel volume using the following equation:

$$V_W = F * \tau_R$$

where F is the combined volumetric flowrate of the inlet stream and τ_R is the space time. The working vessel volume is divided by the "Working / Vessel Volume" parameter to calculate the vessel volume, V. The length of the tube is calculated by dividing the vessel volume by the cross sectional area which is calculated based on the vessel diameter that is always specified by the user. Under rating mode of calculation where the length is specified, the above equations are solved for τ_R .

Material Balances

For a component A that enters a PFR, the component balance equation for a constant density system is given by the following equation:

$$F dC = r_A A dL \quad \text{or} \quad F \int_{C_{in}}^C \frac{dC}{r_A} = AL$$

where F is the feed volumetric flowrate, C_{in} is the inlet concentration, C is the outlet concentration, A is the cross sectional area of the reactor, L is the length of the reactor, and r_A is the combined reaction rate of component A, given by:

$$r_A = \sum_{j=1}^q r_{Aj}$$

where r_{Aj} is the reaction rate of component A due to reaction j and q is the overall number of reactions. If K is the rate reference component of reaction j, then, the reaction rate of component A due to reaction j is given by the following equation:

$$r_{Aj} = \frac{v_{Aj}}{v_{kj}} (r_{kj})$$

where v_{Aj} and v_{kj} are the stoichiometric coefficients of components A and K in reaction j and can be specified on mass or molar basis. Negative stoichiometric coefficients are used for reactants and positive for products. The general rate expression (based on the rate reference component) of a reaction j is given by the following equation:

$$r_j = \frac{k \prod_{i=1}^N (C_i)^{\alpha_i}}{K1 + Cm + Cn / K2}$$

where C_i [kmol/m³] is the concentration of component i [kmol/m³] and α_i is the order of the j th reaction with respect to component i . K_1 and K_2 are user-specified constants. C_m [kmol/m³] and C_n [kmol/m³] are the concentrations of components m and n that are identified by the user. N is the total number of reactions. The reaction rate constant k is either specified by the user or calculated using an Arrhenius expression:

$$k_j = A_j \exp\left(-\frac{E_j}{RT}\right)$$

where A_j is the pre-exponential factor (or frequency factor) and E_j is the activation energy of the j th reaction. **Please be careful when you select the units and specify the values of k_j or A_j .** The units of the overall rate expression must be in kmol/m³-s.

The above equations written for each component entering a PFR constitute a system of ordinary differential equations that are integrated numerically to calculate the composition of the outlet stream.

For systems of variable reaction mixture density (which is often the case for gaseous reactions), the simplified material balance equation cannot be used. An excellent description of the formulation used in that case can be found in the literature (Fogler, 1992 - pp. 505-507).

For a PFR operating in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per batch by the process time and the number of cycles per batch of the reactor unit. The number of cycles (a scheduling parameter) can be set through the Scheduling tab of the step's dialog.

Thermal Mode

A PFR can operate isothermally (at a constant operating temperature), adiabatically (no exchange of heat with the surroundings), or with an evenly distributed heating or cooling duty along the length of the reactor. Under isothermal conditions, the model calculates the heating or cooling requirement along the length of the reactor and stores the values in the profiles (see Profiles below). The heating/cooling duty displayed on the Operating Conditions tab in kcal/h represents averaged values over the whole reactor. Under conditions of specified heating or cooling, the model calculates the temperature of the reacting mixture along the length of the reactor and stores the values in the profiles. Adiabatic operation is a special case of specified heating or cooling duty.

Profiles

The plug flow reaction operation can generate profiles of temperature, heating/cooling duty, and component concentration along the length of the reactor.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated. The working to vessel volume ratio has a default value of 100%. Presence of catalyst or other packing material may result in working to vessel volume ratios of less than 100%.

In Rating Mode, the user specifies the vessel volume, the number of units, and the working to vessel volume ratio and the system calculates the residence time.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

References

Fogler, H. S. 1992. Elements of Chemical Reaction Engineering, 2nd edition, Prentice Hall.

Fermentation Operations

Fermentation (Batch Stoichiometric)

The stoichiometric fermentation model can be used to simulate bio-transformations when the reaction kinetics are unknown or unimportant but the mass stoichiometry is known and the extent of reaction can be specified or calculated based on the concentration of a reference component. The extent of reaction is defined as the fractional conversion of the limiting component. It is possible to have simultaneous feeding of reactants during the reaction, if the Fed Batch options are selected/specified.

Material Balances

The reactions are assumed to occur in a sequence (one after the other). In that sense, the calculations assume that the product mixture of the first reaction is the reacting mixture of the second, and so on. The reactants brought in by the feed stream (in the case that fed batch option is selected) are assumed to be initially present in the reactor as no kinetic considerations are made.

The user provides the mass or molar stoichiometric coefficients (A_i) of the various components for each reaction and the extent of reaction (x) based on either the limiting component or a reference component. Negative stoichiometric coefficients are used for reactants and positive for products. The coefficients can be supplied in either mass or molar units. The algorithm used by the program to perform the material balances for each reaction is explained in the following paragraphs.

If the extent of the reaction is expressed based on the limiting component then, first of all, the limiting component is identified. This is done based on the mass stoichiometry and the composition of the reacting mixture. If the extent of the reaction is expressed based on a user-defined component, then first of all, the program attempts to validate that the user-defined conversion is achievable (i.e., there are enough reactants for the reaction to proceed to such an extent). If that is not the case, then the conversion (x) is adjusted to reflect the maximum achievable conversion percentage (based on the extent-component chosen by the user).

For the limiting component (k) or the extent-reference component (depending on what is the case) the following holds:

$$F_{out_k} = F_{in_k}(1 - x),$$

where,

F_{out_k} is the mass flowrate of the component after the reaction,

F_{in_k} is the mass flowrate of the component before the reaction, and

x is the (possibly adjusted) reaction extent.

Now, the mass flowrate after the reaction (F_{out_i}) of any other component present (i) as a function of its mass flowrate (F_{in_i}) before the reaction, the extent of reaction (x), and the mass stoichiometric coefficients (A_i), is given by the following equation:

$$F_{out_i} = F_{in_i} - F_{in_k} x \left(\frac{A_i}{A_k} \right),$$

where A_k is the coefficient of the limiting or extent-reference component.

The same algorithm is repeated for all reactions specified using the product-mixture of reaction N-1 as the feed of reaction N.

Aeration Rate

When the aeration rate is set by the user (in Volume of air under standard conditions per Volume of fermentation broth per Minute - VVM), the flowrate of the aeration stream is adjusted by the fermentation model. If the aeration stream has a source unit procedure (e.g., a compressor), then the adjustment of its flowrate is recursively back - propagated till flowsheet feed streams are reached. At least one of the flowsheet feed streams that feed into the aeration stream must have non-zero flowrate. Only units with a single output stream can be part of the sequence of units that feed into an aeration stream. An exception to this rule is the "Custom Mixer" which is not allowed to be part of the sequence even though it has a single output stream.

Vapor Emissions

Vapor-liquid equilibrium calculations in the fermentor are not carried out. To account for gas components exiting in the gas outlet stream, the user must specify the removal fraction (Percent in Gas Outlet) for each component. The calculation of the gas outlet stream composition is based on materials that are available in the vessel after the completion of the fermentation.

Intra/Extracellular Component Flowrate

You may also specify the extracellular percent (100% by default) of each of the reaction's product components. This feature is useful when tracking of intracellular water is desired because it affects the performance of centrifugation, filtration, etc. further downstream. If the "Extra-Cell %" of certain reaction product components is less than 100 (or in other words a fraction of the component is intracellular) and the "Primary Biomass" and "Water" components are identified (through the component registration dialog window), then the model automatically associates intracellular water with the intracellular reaction product components. Then, if a separator is used to remove intracellular components (i.e., removal of biomass by a centrifuge), the separation (removal %) of intracellular water will be the same as that of the intracellular component(s).

Utility Calculation

The average agitation power is estimated by multiplying the unit power requirement (kW/m³ of broth) by the liquid volume of the fermentor.

To estimate the overall heating or cooling requirement, the model considers the sensible heat of the inlet and outlet streams along with the heat of reaction. The calculation of the heat of reaction for aerobic systems is based on the oxygen uptake rate (Cooney et. al., 1968):

$$Q_f = 0.12 Q_{O_2},$$

where Q_f is heat release in kcal/L-hr and Q_{O_2} is the oxygen uptake rate in kmol/L-hr. A default value of -3750.0 kcal/(kg of oxygen utilized) is used based on the above model.

Vessel Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

References

Cooney, C. L., D. I. C.Wang, and R. I. Mateles (1968). Measurements of Heat Evolution and Correlation with Oxygen Consumption during Microbial Growth. *Biotechnol. Bioeng.* **11**, 269-281.

Fermentation (Batch Kinetic)

This unit operation model can handle any number of biotransformation reactions and supports a wide variety of fermentation kinetics. A reaction can be initiated at a specific time relative to the beginning of the unit's process time or when the concentration of a certain component exceeds or drops below a certain value. Similarly, a reaction can be terminated at a specific time relative to the end of the unit's process time or when the concentration of a certain component exceeds or drops below a certain value. The contents of the vessel are assumed well mixed at any time point. It is possible to have simultaneous feeding of reactants during the reaction, if the Fed Batch options are selected/specified.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Material Balances

For a component A that reacts in a batch reactor, the generalized component balance is given by the following equation:

$$\frac{dN_A}{dt} = r_A \cdot V + F_0 \cdot x_A$$

where V is volume of material in the reactor, N_A is the amount (mass/moles) of component A, r_A is the combined reaction rate of component A as a function of time, F_0 is the (mass/ molar) flowrate of the feed stream (in the case of simultaneous feeding) and x_A is the (mass /mole) fraction of component A in the feed stream. (If the amount of components is expressed in terms of mass, then F_0 is a mass flow rate and x_A is the mass fraction of component A and if the amount is in moles then F_0 is a molar flow rate and x_A is the mole fraction.)

The (mass / molar) concentration of a component A is given by:

$$C_A = \frac{N_A}{V}$$

In the case of no feed stream (fed batch options are not selected) and constant density system the component balance reduces to:

$$r_A = \sum_{j=1}^q r_{Aj}$$

The reaction rate r_A of component A is given by:

$$r_{Aj} = \frac{v_{Aj}}{v_{kj}}(r_{kj})$$

where v_{Aj} and v_{kj} are the stoichiometric coefficients of components A and K in reaction j and can be specified on mass or molar basis. Negative stoichiometric coefficients are used for reactants and positive for products. The general rate expression (based on the rate reference component) of a reaction j is given by the following equation:

$$r_j = [\alpha \mu_{\max} (S1 - Term)(S2 - Term) + \beta] (B - Term)$$

where α and β are constants, μ_{\max} is the maximum specific biomass growth rate, S1 and S2 terms represent the kinetic expressions of two different components (e.g., substrates or reaction products), and B-Term represents the kinetic expression of the biomass component. The kinetic expression options for S1 and S2 terms include Monod, Haldane (with product inhibition), first order, and none.

The above equations written for each component reacting in a batch fermentor constitute a system of ordinary differential equations, which are integrated numerically to calculate the final composition of the reacting mixture. The integration time is equal to the process time of the unit. A reaction, however, can be initiated or terminated at any time during that time period using the 'Start' and 'End' reaction criteria.

To account for emissions, the user can specify the percentage of each component that is emitted. Please note that the specified percentage is based on the composition of the mixture at the end of the reaction.

Energy Balances

Rigorous energy balances are performed that take into account the heat of reaction and the agitation power (it is assumed that all agitation power dissipates into heat). The model can estimate and record heating or cooling requirement as a function of time (see Profiles further down).

Electricity Consumption

The average agitation power is estimated by multiplying the unit power requirement (kW/m³ of liquid mixture) by the liquid volume.

Profiles

The batch fermentation model can generate profiles of component concentration and heating/cooling duty as a function of time.

References

Fogler, H. S. 1992. Elements of Chemical Reaction Engineering, 2nd edition, Prentice Hall.

Fermentation (Continuous Kinetic)

The continuous fermentation model handles any number of reactions and supports a wide variety of fermentation kinetics. The inlet stream(s) is/are assumed to be perfectly (and instantaneously) mixed with the material already in the reactor, so that the outlet stream composition is identical to that of the reactor contents.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Material Balances

For a component A that enters a continuous fermentor, the component balance equation is given by the following equation:

$$0 = F C_{in} - F C - V_L r_A$$

where F is the volumetric flowrate, C_{in} is the inlet concentration of component A , C is the outlet concentration of component A , and r_A is the combined reaction rate of component A , given by:

$$r_A = \sum_{j=1}^q r_{Aj}$$

where r_{Aj} is the reaction rate of component A due to reaction j and q is the overall number of reactions. If K is the rate reference component of reaction j , then, the reaction rate of component A due to reaction j is given by the following equation:

$$r_{Aj} = \frac{v_{Aj}}{v_{kj}} (r_{kj})$$

where v_{Aj} and v_{kj} are the stoichiometric coefficients of components A and K in reaction j and can be specified on mass or molar basis. Negative stoichiometric coefficients are used for reactants and positive for products. The general rate expression (based on the rate reference component) of a reaction j is given by the following equation:

$$r_j = [\alpha \mu_{\max} (S1 - Term)(S2 - Term) + \beta](B - Term)$$

where α and β are constants, μ_{\max} is the maximum specific biomass growth rate, S1 and S2 terms represent the kinetic expressions of two different components (e.g., substrates or reaction products), and B-Term represents the kinetic expression of the biomass component. The kinetic expression options for S1 and S2 terms include Monod, Haldane (with product inhibition), first order, and none.

The above equations written for each component entering a continuous fermentor constitute a set of non-linear equations, which is solved numerically to calculate the outlet stream concentration.

To account for emissions, the user can specify the percentage of each component that is emitted. Please note that the specified percentage is based on the composition of the outlet stream.

Energy Balances

Rigorous energy balances are performed that take into account the heat of reaction, the agitation power (it is assumed that all agitation power dissipates into heat), and the sensible heat of input and output streams. The model estimates the required heating or cooling duty under certain operating conditions.

Electricity Consumption

The average agitation power is estimated by multiplying the unit power requirement (kW/m³ of liquid mixture) by the liquid volume.

Equipment Purchase Cost

Equipment purchase cost is based on total vessel volume, agitation power and material of construction. The equipment purchase cost includes the cost of the vessel along with the agitator cost. If the vessel is checked as an "ASME Vessel" (i.e., constructed according to standards published by the American Society of Mechanical Engineers) then it is assumed to withstand pressure to 35 psig and its purchase cost is penalized by 20% over the base vessel cost. If the operating pressure of the vessel is set to a pressure higher than 3 atm, then the vessel's purchase cost is penalized by an 80% increase over the base cost.

References

Fogler, H. S. 1992. Elements of Chemical Reaction Engineering, 2nd edition, Prentice Hall.

Environmental Reaction Operations

Well-Mixed (WM) Aerobic BioOxidation

This unit operation model simulates transformation (e.g., bio-oxidation, chemical oxidation, hydrolysis, photolysis, nitrification, sorption, etc.) of organic and other compounds in a well-mixed tank under aerobic conditions. Any number of reactions can be specified with a variety of kinetic expressions. The stoichiometry of a reaction is specified on a mass or molar basis while the reaction rate is specified by selecting appropriate expressions for the substrate term, the other term (e.g., oxygen), and the biomass term. The reaction rate constant is either specified by the user or retrieved from the component databank for biochemical oxidation reactions that follow Monod-type of kinetics. The various reactions may be based on different biomass components. For instance, heterotrophic biomass may be used for biochemical oxidation reactions and autotrophic biomass for nitrification reactions. Biomass death and hydrolysis reactions may be written to keep track of the active and dead fractions of biomass components.

Equipment Sizing

In Design Mode of calculation, the user specifies the hydraulic residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

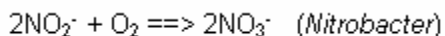
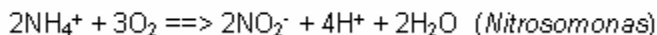
$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated. The tank depth is always specified by the user. Then, using the Length/Width ratio, the program calculates all the dimensions of the tank(s).

In Rating Mode, the user specifies the vessel volume and the working to vessel volume ratio and the program calculates the hydraulic residence time.

Nitrification Reactions

Nitrification is the biological oxidation of ammonia to nitrate with nitrite formation as an intermediate. Nitrification may occur in aeration basins along with other oxidation reactions if the sludge residence time is large enough to prevent wash out of the nitrifying microorganisms. The microorganisms involved are the autotrophic species *Nitrosomonas* and *Nitrobacter*, which carry out the reaction in two steps (Eckenfelder, 1989):



The rate of nitrification has been reported in the literature (Wong-Chong and Loeht, 1975) as essentially constant with overall biomass concentrations (as VSS) up to 1500 mg/l and decreases above that level. An average nitrification rate, at 20 °C, is around 1.04 mg $\text{NH}_3\text{-N}$ oxidized per milligram of nitrifying microbial mass per day. Note that it is easy to express nitrification rates based on nitrifying biomass (autotrophs) if you specify a component (during component initialization) representing nitrifying biomass. Like all biochemical reactions, the rate of nitrification is temperature-dependent with θ in the range of 1.03 to 1.15.

VOC Emissions

The aeration basin model handles VOC emission calculations. Different models exist for surface and diffused aeration that are mass transfer and equilibrium limited, respectively.

Sorption

In terms of sorption, you may specify the fraction of a component that adsorbs on the primary biomass component. The program, then, keeps track of the fraction in solution throughout the flowsheet with the "Extra-Cell %" term. The "Extra-Cell %" term represents the percentage of a component that is in solution while 100 - "Extra-Cell %" represents the adsorbed portion of a component.

Material Balances

For steady-state operation of an aeration basin, the general material balance equation for a component that biodegrades and is emitted is given by the following equation:

$$0 = (\text{Input}) - (\text{Output}) - \left(\begin{matrix} \text{Biochemical} \\ \text{Oxidation} \end{matrix} \right) - \left(\begin{matrix} \text{Surface} \\ \text{Volatilization} \end{matrix} \right) - \left(\begin{matrix} \text{Diffused} \\ \text{Air} \\ \text{Stripping} \end{matrix} \right)$$

$$\text{or} \quad 0 = QC_{in} - QC - Vr_b - K_L aVC - Q_a K_{eq} CF_{st}$$

where Q is the liquid flow rate, V is the reactor volume, C_{in} is the inlet concentration, C is the outlet concentration which is the same as the concentration in the reactor, r_b is the biodegradation rate, $K_L a$ is the overall mass transfer coefficient, Q_a is the air flow rate (in case of diffused aeration), K_{eq} is the equilibrium constant, and F_{st} is the saturation term (it represents the extent of saturation of the exiting gas stream). In general, the biodegradation rate is a function of substrate concentration, oxygen concentration, and biomass concentration. Various expressions are available for the effect of substrate. The overall equation with a Monod-type substrate expression is written as follows:

$$r_b = K_{max} \left(\frac{C}{K_s + C} \right) \left(\frac{C_o}{K_o + C_o} \right) X$$

where K_{max} is the maximum rate constant, K_s is the half saturation constant for the substrate, C_o is the oxygen concentration, K_o is the half saturation constant for oxygen, and X is the biomass concentration. Alternative expressions for the substrate and oxygen terms are also available. The component databank includes data for K_{max} and K_s for a large number of chemical components.

The overall mass transfer coefficient of a VOC component is estimated as a function of the oxygen mass transfer coefficient in wastewater, using a proportionality coefficient, ψ_M . In other words,

$$(k_1 a)_{VOC} = \psi_M (k_1 a)$$

The value of $(K_L a)_{O_2}$ in the wastewater is a user input to the program. ψ_M is given by the following equation (Hsieh et. al., 1993):

$$\psi_M = \psi \left\{ 1 + \frac{1}{H_c \frac{k_g a}{k_l a}} \right\}^{-1}$$

ψ is the dimensionless transfer coefficient proportionality constant and it is calculated by the following equation (Corsi and Card, 1991):

$$\psi = \left\{ \frac{D_{voc}}{D_{O_2}} \right\}^n$$

where D_{voc} and D_{O_2} are the liquid diffusion coefficients for a VOC and oxygen in (m^2/s), respectively. The exponent n varies from 0.5 for penetration and surface renewal theories to 1.0 for two-film theory (Corsi and Card, 1991) and is typically 0.5 to 0.6 (Mihelcic et. al., 1993). The diffusion coefficients of VOC components are retrieved from the component databank of the program.

$k_g a$ and $k_l a$ are the individual mass transfer coefficients of the VOC in the gas and liquid phases, respectively, in (s^{-1}). For mechanically aerated systems, the value of $\frac{k_g a}{k_l a}$ is estimated using the following empirical equation (Hsieh et. al., 1993):

$$\log \left(\frac{k_g a}{k_l a} \right) = -0.39664 \log_{10} (P / V) + 2.6776$$

(P/V) represents the mechanical power consumed for surface aeration divided by the liquid volume of the aeration basin and it is calculated by the program. Alternatively, you have the option to set the value of $k_g a/k_l a$ or set the value of the term in parenthesis (denoted by RI/Rt on the emission i/o dialog window).

For diffused aerated systems, the F_{st} term is calculated by the following equation:

$$F_{st} = 1 - \exp \left(\frac{\psi_M (K_L a)_{O_2} V}{H_c Q_g} \right)$$

To calculate ψ_M , you have the option to set either the $k_g a/k_l a$ ratio or the term in parenthesis (called RI/Rt on the emission i/o dialog window).

The equilibrium constant is estimated by:

$$K_{eq} = \frac{H_c}{RT}$$

where H_c is Henry's law constant, R is the universal gas constant, and T is temperature.

The above equations written for each chemical component entering an aeration basin constitute a set of non-linear equations, which is solved numerically to calculate the exit concentration and the emission rate of each component.

References

1. Corsi, R. L., and T. R. Card. 1991. "Estimation of VOC Emissions Using the BASTE Model," *Environmental Progress*. 10: 290-299.
2. Eckenfelder, W.W., Jr., 1989, Industrial Water Pollution Control, McGraw-Hill, NY.
3. US EPA, 1975, Process Design Manual for Nitrogen Control.
4. Hsieh, C.-C., K. S. Ro, and M. K. Stenstrom, "Estimating Emissions of 20 VOCs. I: Surface Aeration, II: Diffused Aeration", *J. of Env. Engr.*, Vol. 119, No. 6, Nov./Dec. 1993, ASCE, ISSN 0733-9372.
5. Mihelcic, J. R., C. R. Baillod, J. C. Crittenden, and T. N. Rogers. 1993. "Estimation of VOC Emissions from Wastewater Facilities by Volatilization and Stripping," *Journal of Air and Waste Management Association*. 43: 97-105.
6. Melcer, H, J. P. Bell, D. J. Thomas, C. M. Yendt, J. Kemp, and P. Steel. 1994. "Modeling Volatile Organic Contaminants' Fate in Wastewater Treatment Plants," *Journal of Environmental Engineering*. 120: 588-609.
7. Melcer, H. 1994. "Monitoring and Modeling VOCs in Wastewater Facilities," *Environmental Science and Technology*. 28: 328A-335A.
8. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", Third edition, Metcalf & Eddy, Inc., McGraw-Hill, Sec. 10-1.
9. Wong-Chong, G.M., and R.C. Loeht: *Water Res.*, vol. 9, p. 1099, 1975.

Plug-Flow (PF) Aerobic BioOxidation

The Plug Flow Aerobic BioOxidation (PFAB) model can simulate any number of parallel or sequential reactions that may represent biochemical oxidation, hydrolysis, chemical oxidation, photolysis, nitrification, etc. The PFAB model assumes that axial mixing is negligible.

Equipment Sizing

In Design Mode of calculation, the user specifies the hydraulic residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated. The tank depth is always specified by the user. Then, using the Length/Width ratio, the program calculates all the dimensions of the tank(s).

In Rating Mode, the user specifies the vessel volume and the working to vessel volume ratio and the program calculates the hydraulic residence time.

Material Balances

For a component A that enters a PFAB unit, the component balance equation is given by the following equation:

$$F dC = r_A A dL \text{ or } F \int_{C_{in}}^C \frac{dC}{r_A} = AL$$

where F is the feed volumetric flowrate, C_{in} is the inlet concentration, C is the outlet concentration, A is the cross sectional area of the liquid flow, L is the total liquid flow length in the reactor (it depends on the number of compartments and the orientation of the compartments), and r_A is the combined reaction rate of component A, given by:

$$r_A = \sum_{j=1}^q r_{Aj}$$

where r_{Aj} is the reaction rate of component A due to reaction j and q is the overall number of reactions. If k is the rate reference component of reaction j , then, the reaction rate of component A due to reaction j is given by the following equation:

$$r_{Aj} = \frac{v_{Aj}}{v_{kj}} (r_{kj})$$

where v_{Aj} and v_{kj} are the stoichiometric coefficients of components A and k in reaction j and can be specified on mass or molar basis. Negative stoichiometric coefficients are used for reactants and positive for products. The general rate expression (based on the rate reference component and for Monod-type of substrate expressions) of a reaction j is given by the following equation:

$$r_j = K_{\max} \left(\frac{C}{K_s + C} \right) \left(\frac{C_o}{K_o + C_o} \right) X$$

where K_{\max} is the maximum rate constant, K_s is the half saturation constant for the substrate, C_o is the concentration of a second substrate component (e.g., oxygen), K_o is the half saturation constant for the other substrate component, and X is the biomass concentration. Alternative expressions for the substrate and second substrate terms are also available. The component databank includes data for K_{\max} and K_s for a large number of chemical components.

The above equations written for each component entering a PFAB unit constitute a system of ordinary differential equations which are integrated numerically to calculate the composition of the outlet stream.

Sorption and VOC Emissions

Sorption and VOC emissions initialization and calculations are identical to those of the Aeration Basin.

References

1. Corsi, R. L., and T. R. Card. 1991. "Estimation of VOC Emissions Using the BASTE Model," *Environmental Progress*. 10: 290-299.
2. Eckenfelder, W.W., Jr., 1989, *Industrial Water Pollution Control*, McGraw-Hill, NY.

Anaerobic Digestion

Process Description

Anaerobic digestion is one of the oldest processes used for the stabilization of sludges. It involves the decomposition of organic and inorganic matter in the absence of molecular oxygen. The major applications have been, and remain today, in the stabilization of concentrated sludges produced from the treatment of wastewater and in the treatment of some industrial wastes. More recently, it has been demonstrated that dilute organic wastes can also be treated anaerobically (Tchobanoglous and Burton, 1991).

Anaerobic digestion utilizes airtight tanks in which anaerobic microorganisms stabilize the organic matter producing methane, carbon dioxide and other end products.

Organic matter \rightarrow CH_4 + CO_2

Roughly four groups of microorganisms sequentially degrade organic matter. Hydrolytic microorganisms degrade polymer-type material such as polysaccharides and proteins to monomers. The monomers are then converted into fatty acids with a small amount of H_2 . The principal acids are acetic, propionic, and butyric with small quantities of valeric. All acids higher than acetic acid are converted into acetate and H_2 , by acetogenic microorganisms. The acetic acid and H_2 are converted to CH_4 by methanogenic organisms (Eckenfelder, 1989).

There are two main types of anaerobic digesters, standard rate and high rate. In the standard-rate digestion process, the digester contents are usually unheated and unmixed. The digestion period may vary from 30-60 days. In a high-rate digestion process, the digester contents are heated and completely mixed. The required detention period is 10-20 days.

The digester gas contains approximately 60-70% methane, 25-30% carbon dioxide and small amounts of hydrogen, nitrogen, hydrogen sulfide, and other gases. The gas has a heating value of 21,000-25,000 kJ/m^3 .

The hot water or steam used to heat digesters is most commonly generated in a boiler fueled by digestion gas. Up to 80% of the gas heating value can be recovered in a boiler. Additional heating (if required) is provided by natural gas.

Model Description

The anaerobic digester is modeled as a well-mixed reactor with kinetics. Any number of reactions can be specified that represent various types of reactions. The stoichiometry of a reaction can be specified on a mass or molar basis while the reaction rate is specified by selecting appropriate expressions for the substrate term, the oxygen term, and the biomass term. You may either specify the reaction rate constant of each reaction at the actual operating temperature or at a reference temperature. If the rate constant is specified at a reference temperature, the parameter "Theta" that affects the calculation of the rate constant at any temperature must be specified too.

The reaction rate initialization interface offers flexibility in specifying a great variety of kinetic expressions. If, for instance, an average overall reaction rate is available for a certain type of industrial waste, it can be specified as the value of K with the "None" option selected for the substrate, oxygen, and biomass terms. Such overall reaction rate data are available for several industrial wastes (Eckenfelder, 1989, pp. 249, 256).

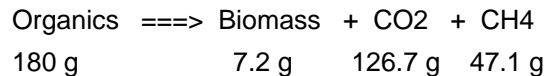
For sludge stabilization, the values of rate constants are usually in the following ranges.

$K = 0.010 - 0.020 \text{ 1/h}$ (for hydrolytic and catabolic reactions)

$K_S = 8,000 - 12,000$ mg/liter (for hydrolytic and catabolic reactions)

$K_D = 5 \times 10^{-4} - 7 \times 10^{-4}$ 1/h (for active biomass decay reactions)

The yield coefficient, Y [g biomass / g substrate] is usually in the range of 0.04 - 0.06. This information is useful in specifying the stoichiometry of a degradation reaction. An example of such a reaction follows:



Specify the "Gas Release %" to account for gaseous components exiting in the gas outlet stream. Similarly, the "Sorption %" determines the percentage of a component that adsorbs on the primary biomass component. The program, then, keeps track of the fraction in solution throughout the flowsheet with the "Extra-Cell %" term. The "Extra-Cell %" term represents the percentage of a component that is in solution while $100 - \text{"Extra-Cell \%"} represents the adsorbed portion of a component.$

Use the "Heating Agent" variable to specify the utility used (e.g., natural gas, steam, etc.) for heating up the unit in the case of a high-rate digester.

Equipment Sizing

In Design Mode of calculation, the user specifies the hydraulic residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated. The tank depth is always specified by the user. Then, using the Length/Width ratio, the program calculates all the dimensions of the tank(s).

In Rating Mode, the user specifies the vessel volume and the working to vessel volume ratio and the program calculates the hydraulic residence time.

References

1. Eckenfelder, W.W., Jr., 1989, Industrial Water Pollution Control, McGraw-Hill, NY.
2. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", Third edition, Metcalf & Eddy, Inc., McGraw-Hill, Sec. 6-8.
3. Qasim S. R. (1994). "Wastewater Treatment Plants: Planning, Design and Operation", Technomic Publishing Co., Inc., Basel, Switzerland

Trickling Filtration

Process Description

A trickling filter is a packed bed of media covered with slime growth over which wastewater is passed. As the waste passes through the filter, organic matter present in the waste is removed by the biological film (Eckenfelder, 1989).

Plastic packings are employed in depths up to 12.2 m (40 ft), with hydraulic loadings as high as $0.16 \text{ m}^3/\text{m}^2\text{-min}$ ($4.0 \text{ gal/ft}^2\text{-min}$). Depending on the hydraulic loading and depth of the filter, BOD removal efficiencies as high as 90% have been attained on some wastewaters.

Material Balances and Equipment Sizing

In terms of material balances, the trickling filter is modeled as a stoichiometric reactor. The user provides the stoichiometry and the extent of reaction (based on a limiting or reference component) for any number of biochemical oxidation and other type of reactions.

In Design Mode of calculation, one of two models can be utilized to size the trickling filter:

The National Research Council (NRC) model is based on the data analysis of stone media trickling filter plants. It considers that the contact between the filter media and organics depends on the filter dimensions. The filter volume V is given by the following equation:

$$V = \frac{0.000196 Q S_i}{R_f} \left[\frac{E}{1 - E} \right]^2$$

where: E = fraction of BOD_5 removed
 Q = influent flowrate (m^3/day)
 S_i = influent BOD_5 (mg/l)
 R_f = recycle factor defined by:

$$R_f = \frac{1 + \alpha}{[1 + (1 - \delta)\alpha]^2}$$

where: δ = weighing factor value (typical value = 0.9)
 α = recycle ratio (recirculation flow / influent flow)

The above equation is used to calculate the required volume, V , of the trickling filter. The specified hydraulic loading (in $\text{m}^3/\text{m}^2\text{-day}$) along with the recycle ratio are used to calculate the required cross sectional area, A . Then, the depth of the filter is calculated by dividing the volume by the area.

The Eckenfelder Model assumes that the trickling filter can be represented as a plug flow reactor and the substrate utilization follows first order kinetics:

$$\frac{S_e(1 + \alpha)}{S_i + \alpha S_e} = \exp \left[-K_o D \left(\frac{A}{(1 + \alpha)Q} \right)^n \right]$$

where,

- S_e is the effluent BOD₅ (mg/l)
- S_i is the influent BOD₅ (mg/l)
- D is the depth of filter media (m)
- A is the cross sectional area of filter (sq.m)
- n a model-constant
- K_o is the treatability factor (1/day)

The constant, n , and the treatability factor, K_o , are functions of the packing media. The program provides values for six different media types (the values of K_o are for 20 °C). The temperature correction factor ($\theta = 1.035$) is used to correct the treatability factor for temperatures different from 20 °C using the following equation.

$$K_{o \text{ (at } T)} = K_{o \text{ (at } 20^\circ\text{C)}} \theta^{(T-20)}$$

The Eckenfelder equation is solved for D , to calculate the required depth of the filter. The cross sectional area, A , is calculated based on the hydraulic loading rate and the recycle ratio. Then, the filter volume is calculated by multiplying the cross sectional area by the depth of the filter.

If the calculated cross sectional area is greater than the area that corresponds to the maximum diameter, then the model assumes multiple filters operating in parallel.

VOC Emission Calculations

Emissions of VOCs from trickling filters occur due to stripping caused by natural or forced air ventilation. The trickling filter is modeled as a packed-media (Corsi and Card, 1991). The emission calculations follow (they are done after) the biodegradation material balances.

The mass balance for a particular VOC around a trickling filter operating countercurrently is written as follows:

$$Q(C_{\ell, \text{in}} - C_{\ell, \text{out}}) = Q_g(C_{g, \text{out}} - C_{g, \text{in}})$$

where Q is the wastewater flowrate in (m³/s) and Q_g is either the natural or forced air ventilation rate, or aeration rate, in (m³/s). $C_{\ell, \text{in}}$ and $C_{\ell, \text{out}}$ are the influent and effluent concentrations of the VOC in the wastewater in (g/m³), respectively. $C_{g, \text{in}}$ and $C_{g, \text{out}}$ are the initial and final concentrations of the VOC in the air in (g/m³), respectively. Since the initial concentration of the VOC in the circulating air is zero, $C_{g, \text{in}}$ is zero, and the above equation becomes:

$$Q(C_{\ell, \text{in}} - C_{\ell, \text{out}}) = Q_g C_{g, \text{out}}$$

Corsi and Card (1991) also make the assumption that the VOCs in the effluent air stream are in thermodynamic equilibrium with VOCs in the influent wastewater stream, or

$$C_{g, \text{out}} = H_c C_{\ell, \text{in}}$$

where H_c is the dimensionless Henry's constant. The combination of the above two equations yields

$$Q(C_{\ell,\text{in}} - C_{\ell,\text{out}}) = Q_g H_c C_{\ell,\text{in}}$$

The above equation is solved for $C_{\ell,\text{out}}$ to calculate the concentration of VOC components in the gas outlet stream. The term $Q(C_{\ell,\text{in}} - C_{\ell,\text{out}})$ represents the rate of VOC emissions from a trickling filter.

References

1. Benefield, L.D. and Randall, C.W. 1980, Biological Process Design for Wastewater Treatment, Prentice Hall.
2. Corsi, R. L., and T. R. Card. 1991. "Estimation of VOC Emissions Using the BASTE Model," *Environmental Progress*. 10: 290-299.
3. Eckenfelder, W.W., Jr., 1989, Industrial Water Pollution Control, McGraw-Hill, NY.
4. Water Pollution Control Federation, 1982, Wastewater Treatment: Plant Design, WPCF Manual of Practice No 8, Lancaster Press, PA.

Neutralization

Many industrial wastes contain acidic or alkaline materials that require neutralization prior to discharge to receiving waters or prior to chemical or biological treatment. For biological treatment, pH in the biological system should be maintained between 6.5 and 8.5 to ensure optimum biological activity. Usually neutralization processes work better with the stepwise addition of reagents.

Material Balances

The neutralizer is modeled as a stoichiometric reactor. The excess (%) of the neutralizing agent is based on the stoichiometrically required amount and is used to adjust the flowrate of the neutralizing agent stream. If multiple components need to be neutralized, the user must specify the neutralization reactions for each of them. The extent of reaction represents the fractional conversion of the limiting or reference component. Note that the neutralizing agent (specified on the Operating Conditions tab) cannot be the reference component of a neutralization reaction.

Equipment Sizing

In terms of equipment sizing, this unit models a multi-stage (multi-tank) operation. The number of neutralization stages is always specified by the user. Then, in design mode, the user specifies the residence time of the liquid in the system (including all stages) and the program calculates the liquid volume of each stage and the number of parallel tank chains. In rating mode, the user specifies the vessel volume of each stage, the number of parallel tank chains, and the working to vessel volume ratio and the program calculates the residence time of the liquid in the system.

VOC Emission Calculations

For volatile organic compound (VOC) emission calculations, it is assumed that the neutralizer behaves like a quiescent tank. The calculations are identical to those of the Clarification Model.

References

Eckenfelder, W.W., Jr., 1989, Industrial Water Pollution Control, McGraw-Hill, NY.

Wet-Air Oxidation

Wet oxidation is an aqueous-phase oxidation process brought about when an organic and/or oxidizable inorganic-containing liquid is mixed thoroughly with a gaseous source of oxygen (usually air) at temperatures of 150 to 325 °C. Gauge pressures of 20 to 210 bar (300 to 3,000 psi) are maintained to promote reaction and control evaporation (Copa and Gitchel, 1988).

In wastewater treatment, wet oxidation in the temperature range of 150 to 200 °C improves sludge dewaterability. Intermediate temperatures of 200 to 280 °C are used in such applications as spent activated-carbon regeneration and conversion of refractories to biodegradable substances. Still higher temperatures (280 to 325 °C) provide essentially complete oxidation. Residence times of 15 to 60 min are required for 95 to 99 % oxidation. Adjustment of pH, especially to lower values, accelerates rates.

In most cases where wet oxidation is applied to hazardous wastes, the treatment objectives are the detoxification of the wastewater for subsequent biological treatment, which can be accomplished in a publicly owned treatment works (POTW) facility or an industrial treatment plant. Wet oxidation is very effective in treating wastes containing inorganic and organic cyanides and sulfides at temperatures less than 250 °C and gauge pressures below 140 bar. Wastes containing halogenated aromatic compounds with at least one non-halogen functional group, e.g., pentachlorophenol or 2,4,6-trichloroaniline, are effectively treated by wet oxidation at temperatures of 250 to 320 °C and gauge pressures of up to 205 bar.

The wet oxidation unit is modeled in this program as a stoichiometric reactor. The user specifies the stoichiometry of oxidation reactions on a mass or molar basis. The extent of reaction represents the fractional conversion of the limiting or reference component. The oxygen supply (usually in the form of air) is adjusted by the model based on the excess % that is specified by the user. The excess amount of oxygen is calculated based on the stoichiometrically required amount.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time of the liquid in the system and the program calculates the vessel volume and the number of units. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated. In Rating Mode, the user specifies the volume and the number of vessels and the program calculates the residence time of the liquid in the system.

References

1. Copa, W.M. and W.B. Gitchel, 1988, "Wet Oxidation" in 'Standard Handbook of Hazardous Waste Treatment and Disposal', Harry M. Freeman (ed), McGraw-Hill, pp. 8.77 - 8.90.

Incineration

The unit operation model simulates incineration of wastewater sludges, hazardous wastes (liquid or solid), and municipal solid wastes. The primary objective of the model is to calculate the composition of the flue gas stream and estimate the flowrate of auxiliary fuel if needed.

Material and Energy Balances

The user specifies the elemental composition of all chemical components that are present in the feed streams (waste feed, fuel feed, and air inlet streams). The elemental composition in mass % includes the following elements/components: (i) Carbon, (ii) Hydrogen, (iii) Moisture, (iv) Oxygen, (v) Nitrogen, (vi) Chlorine, (vii) Fluorine, (viii) Bromine, (ix) Iodine, (x) Sulfur, (xi) Phosphorus, and (xii) Ash. The user must also identify the following components (that may be present in the flue gas stream): carbon dioxide, water, nitrogen, oxygen, hydrogen chloride, hydrogen fluoride, bromine, iodine, sulfur dioxide, phosphorous pentoxide, and ash. The following assumptions are made in the material balance calculations:

1. All carbon in the feed streams will be converted to carbon dioxide.
2. All hydrogen will be oxidized to water and if chlorine and/or fluorine are present, then, stoichiometric amounts of hydrogen will be used to convert the halogens into hydro-halogens.
3. All nitrogen contained in combustible components will be released as gaseous N_2 .
4. All bromine or iodine present will be released as gaseous Br_2 , I_2 .
5. All sulfur will be converted to sulfur dioxide.
6. All phosphorous will be converted to phosphorous pentoxide (P_2O_5) and
7. All ash will be released as ash.

The model first checks whether the waste feed stream can be burned autothermally at the specified excess oxygen % and flue gas temperature. If yes and the "Adjust Fuel Flow..." button is checked, then, the fuel flowrate is set to zero. If no and the "Adjust Fuel Flow..." button is checked, the required fuel flow is calculated and the fuel stream flowrate is adjusted accordingly. If the "Adjust Fuel Flow..." button is not checked, then, the model checks whether the combined waste feed and fixed fuel feed streams can be burned autothermally. If no, a warning is displayed and material balance calculations are skipped.

In the energy balance calculations, the flue gas temperature that is specified by the user is assumed to be the temperature of the gas stream at the exit of the energy recovery unit. In other words, the model assumes some energy recovery by default.

The flowrate of the air (oxygen) inlet stream is always adjusted by the model based on the "Excess Oxygen %" specified by the user. The user must make sure that the composition of the oxygen supply stream is correctly specified.

Equipment Purchase Cost

The capital cost estimation data are based on multiple-hearth incinerators used for burning wastewater sludge (EPA, 1979). If you need to model and cost incinerators of different designs (e.g., fluidized bed, rotary kiln, etc.), you may want to specify your own capital cost data.

References

1. Theodore L. and J. Reynolds (1987), "Introduction to Hazardous Waste Incineration", John Wiley & Sons.
2. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", 3rd edition, Metcalf & Eddy, Inc., McGraw-Hill, Sec. 12-15.
3. EPA 625/1-79-011 (1979). "Process Design Manual for Sludge Treatment and Disposal", Chapter 9.

UV Radiation

UV Radiation is used in water purification processes to kill microorganisms (Meltzer, 1993). The most common method of generating UV radiation is by discharge lamps. The germicidal effectiveness of UV radiation is dependent upon its wavelength. Different organisms show slightly different sensitivities to various parts of the UV spectrum. The maximum appears to be at a wavelength of around 265 nm. UV radiation also contributes to TOC removal through its generation of free radicals in water.

Disinfection action is dependent not only upon the UV emission spectrum, but also upon the radiation intensity, the duration of the organism exposure, the sensitivity of the organism involved, and the UV transmission of the medium that suspends the organisms.

UV devices are rated by their capacities to treat water at specific flowrates. Actually, the UV dosage is the real consideration. It is the product of radiation intensity and the exposure time, and is expressed as microwatts-seconds per square centimeter ($\mu\text{Ws}/\text{cm}^2$). The time/dose dependency is usually based upon a 10-second dosage. The dwell time in the reactor is specified by the UV lamp manufacturer. As stated, organism elimination by UV radiation is a matter of log reductions: it is not a matter of absolute organism kills. Most reactors are designed for 6-log reductions of organisms.

Ultraviolet lamp life is normally from 500 to 8,000 hours. Lamps deteriorate as a result of solarization (crystallization), or from becoming fouled.

Material Balances

To handle material transformations (e.g., death of microorganisms, destruction of organic compounds, etc.) the user can specify any number of stoichiometric reactions.

Power Consumption

Power consumption is estimated based on the power of each lamp that the user can specify. Alternatively, the user can specify the total power per unit, which typically includes several lamps.

Equipment Sizing

In Design Mode of calculation, the program calculates the operating throughput (in L/min) and if it is greater than the maximum throughput that a unit can handle, it assumes multiple units operating in parallel.

Equipment Capacity Utilization

In Rating Mode, the program divides the operating throughput by the equipment's rated throughput to estimate the equipment capacity utilization.

References

Meltzer, T.H. (1993). "High Purity Water Preparation for the Semiconductor, Pharmaceutical, and Power Industries", Tall Oaks Publishing, Littleton, Colorado.

Charge – Transfer - Pull Operations

Charge

The modeling equations of a Charge operation are very simple. The only goal is to determine the Charge time or Charge rate using the following equation:

$$\text{Time} = \text{Amount} / \text{Flowrate}$$

If the duration of this operation is matched up to another operation (master operation), then the setup time, process time and turnaround time are simply derived from the master operation.

This operation may result in **VOC Emissions** if volatile compounds are involved.

Transfer In

The modeling equations of a Transfer In operation are very simple. The only goal is to determine the transfer time or transfer rate using the following equation:

$$\text{Time} = \text{Amount} / \text{Flowrate}$$

If the duration of this operation is matched up to another operation (master operation), then the setup time, process time and turnaround time are simply derived from the master operation.

This operation may result in **VOC Emissions** if volatile compounds are involved.

Pull In

A Pull-In operation is a superset of the **Charge** and **Transfer In** operations with additional options. The calculations of this model depend on which “Amount Option” is selected. If the “Available In Input Stream” amount option is chosen the operation is identical to a Charge or Transfer In operation and the calculations are performed as in **Charge Model** if the selected pull in stream is an input stream and as in the **Transfer In Model** if the selected pull in stream is an intermediate stream.

Pull In Model Description for the remaining options:

For the rest of the (Amount) options the amount of material is not specified in the input stream but is either set by user directly or computed during the simulation. In the later case model is quite unique in the following way: While the majority of models in Pro-Designer combine variables from input streams and/or the state of the unit procedure (before the operation is executed) with operating conditions and compute variables describing the state of the unit procedure (after the operation) and output streams, this operation operates in reverse: It consults the state of the unit procedure currently and a user's specification possibly regarding the final state of the unit procedure (after the operation is executed) and then modifies the amount of material on the manipulated (pull-in) stream, so that the expressed design objective is met.

Oftentimes, during the design of a new process, it is required to transfer into a vessel (using an intermediate stream) or charge into a vessel (using a process input stream) a certain amount of material in order to meet certain specification of the final mixture in the vessel (e.g. achieve a desired total amount in the vessel). In such cases, the user does not know the amount of material to be brought into the vessel directly but it is to be determined by the program during simulation. This model allows users to express such process design constraints directly. Note that the composition of the adjustable stream (pull-in stream) must be set by the user before the simulation starts, if the stream happens to be a process input stream. The designer can choose to specify one of the following targets (any one of these will determine the amount of material that will be pulled-in):

- a. Specify Mass of the pull-in stream
- b. Specify Volume of the pull-in stream
- c. Specify properties of the final mixture:
 - I. Ratio of pull-in mass or volume to the initial amount
 - II. Final Mass or Volume of the mixture (after the pull-in) operation
 - III. Concentration or mass fraction of a specific component in the final mixture

For case (c) (I, II, III) the flow of the pull-in stream is calculated in an iterative way. Heat and Mass balances are performed in order to determine the final mixture composition and/or the pull-in stream flow rate. The required flow of the pull-in stream, whether set by the user or computed, is propagated backwards, through the network of connectivity. Since iterative calculations are performed, and since the user may have set un-achievable goals in (c) above, it is possible that the model will fail to determine a value for the flow of the adjustable pull-in stream that will meet the matches the user's request. In that case, a warning will message will appear, explaining why the design goal set is unachievable and offering suggestions on how to remedy the situation.

Duration:

If the duration of this operation is matched up to another operation (master operation), then the setup time, process time and turnaround time are simply derived from the master operation.

This operation may result in **VOC Emissions** if volatile compounds are involved.

Pull Out

The modeling equations of a Pull-Out operation are very simple. However, this model is quite unique in the following way: While the majority of models in Pro-Designer combine variables from input streams and/or the state of the equipment (before the operation is executed) with operating conditions and compute variables describing the state of the equipment (after the operation) and output streams, this operation operates in reverse: It consults the amount of material demanded at the output stream associated with it (the pull-out stream, an output stream) and it modifies the content of the vessel such that the contents before and after differ by exactly that amount. Since the operation raising the demand for material that is to be satisfied by this pull-out operation is downstream, the solution engine will visit this operation before it visits the material-demanding operation. Therefore, during the first pass of the solution, the pull-out operation will not consider the correct amount demanded. However, Pro-Designer uses a sophisticated back-propagation scheme that will correct the situation as soon as the downstream operation is reached. When that happens, and as soon as the correct demand is computed, it is propagated backwards, through the network of connectivity, until it reaches:

- (a) A pull-out operation in a vessel, or
- (b) An input streams while the 'auto-adjust' flag turned on.



Tip

If the solution engine never encounters such an operation (that will trigger a backwards propagating scheme) the pull-out operation will remain inactive. In other words, the operation will send on to the output stream whatever amount happened to be from the previous run.

Transfer Out

The modeling equations of a Transfer Out operation are very simple. The main goal is to determine the transfer time or transfer rate using the following equation:

$$\text{Time} = \text{Amount} / \text{Flowrate}$$

If the duration of this operation is matched up to another operation (master operation), then the setup time, process time and turnaround times are simply derived from the master operation.

The material balances are done based on the amount (specified on a percent or absolute basis) that is transferred out.

If, on the emissions tab, the "Saturate Gas Space with VOCs" button is checked, the freeboard space that is created due to transfer out is filled with air that is saturated in VOCs that are present in the liquid mixture that was removed. This may affect the emissions of subsequent operations.

Miscellaneous Vessel Operations

Cool (in a Vessel)

Several cooling options are available in this model. The cooling time can either be set or calculated. When calculated it can be based on a constant cooling or exponential type where the overall heat transfer coefficient is specified

Cooling Time

If the user sets the cooling time (t_p) or a constant cooling rate (dT/dt) the following equation is used:

$$\Delta T = \frac{dT}{dt} t_p$$

Where ΔT is the final temperature minus the initial. When the user specifies the constant heating rate, the above equation is solved for heating time and vice versa.

If an exponential cooling type is chosen, then the user sets the overall UA (kcal/h-°C) and the following equations are used to calculate cooling time:

$$T = T_{c0}(1 + \beta e^{-\alpha t_p})$$

$$\beta = \frac{T_0 - T_{c0}}{T_{c0}}$$

$$\alpha = \frac{WC_p'}{MC_p}(1 - e^{-(UA/WC_p')})$$

where T_{c0} is the inlet temperature of the cooling agent, T_0 is the initial temperature of the vessel contents, MC_p is the sum of the the vessel contents heat capacity and the equipment heat capacity (kcal/°C), W is the flow rate of the cooling agent (kg/min), and C_p' its heat capacity (kcal/kg-°C).

Energy Balance

For all cooling options, and if the cooling agent is not ignored, the average cooling duty (Q) or power (P) is calculated using the following equations:

$$\dot{Q} = P = MC_p \frac{|\Delta T|}{t_p} / \eta$$

where η is the cooling efficiency

Heat (in a Vessel)

Several heating options are available in this model, using a heat transfer agent or electricity. If electricity is used for heating, the heating rate is assumed to be constant and the user can choose between setting the heating time or the heating rate. If a heating transfer agent is used an additional option for setting an exponential type of heating rate is also available (indirect heating).

Heating Time

If the user sets the heating time (t_p) or a constant heating rate (dT/dt) the following equation is used:

$$\Delta T = \frac{dT}{dt} t_p$$

Where ΔT is the final state temperature minus the initial. When the user specifies the constant heating rate, the above equation is solved for heating time and vice versa.

If an exponential heating type is chosen, then the user sets the overall UA (kcal/h-°C) and the following equations are used to calculate heating time:

$$T = T_H (1 + \beta e^{-\alpha t_p})$$

$$\beta = \frac{T_0 - T_H}{T_H}$$

$$\alpha = \frac{UA}{MC_p}$$

where T_H is the inlet temperature of the heating agent, T_0 is the initial temperature of the vessel contents, and MC_p is the sum of the the vessel contents heat capacity and the equipment heat capacity (kcal/°C).

Energy Balance

For all heating types the heating agent is not ignored, the average heat transfer rate (Q) or power (P) is calculated using the following equations:

$$\dot{Q} = P = MC_p \frac{\Delta T}{t_p} / \eta$$

where η is the heating efficiency

This operation may result in **VOC Emissions** if volatile compounds are present in the vessel.

Clean-in-Place (CIP)

The primary objective of this model is to calculate the amount of material used for cleaning a piece of equipment. This is done based on one of the following five specification options:

- ⇒ The cleaning agent rate (in L/min)
- ⇒ The agent's specific volume (in L per equipment size); the units of "size" are equipment specific (e.g., m³ for a vessel, m² for a membrane filter, etc.).
- ⇒ The cleaning agent's total volume (in L)
- ⇒ The cleaning agent's rate per unit of circumference (L/min-m); this option is only available if the operation takes place in a vertical or horizontal vessel or other similar vessel that features a circular cross sectional area.
- ⇒ The cleaning agent's rate per unit of internal surface (L/min-m²); this option is only available in horizontal and vertical vessels.

Please note that the "cleaning agent rate" is the net flowrate and not the recirculating flowrate.

To represent a typical industrial CIP operation, you can use multiple steps for example washing with process water, rinsing with acidic solution, rinsing with caustic solution and rinsing with purified water. You can specify the different parameters for each cleaning step.

The duration of each step is user-specified. The cleaning agent can be selected from the list of registered pure components or stock mixtures. This operation is supposed to be used for cleaning empty equipment items. If material is present in the equipment, the program generates a warning. If the intended use is to remove material from a vessel using a solvent, you should use a Charge operation instead.

A CIP skid can be associated with this operation. If the same skid is utilized by other operations, the program makes sure that the processing times of those operations do not overlap.

Steam-in-Place (SIP)

The primary objective of this model is to calculate the amount of steam used for cleaning a piece of equipment. This is done based on the steam rate (in kg/h) or its amount (in kg) that are specified by the user. The "Cleaning Steam" is selected from the list of available heating agents.

The duration of the operation is specified by the user. This operation is supposed to be used for cleaning empty equipment items. If material is present in the equipment, the program generates a warning.

A SIP skid can be associated with this operation. If the same skid is utilized by other operations, the program makes sure that the processing times of those operations do not overlap.

Pressurize

The primary objective of this model is to calculate the amount of required gas for pressurizing a vessel. The gas is selected from the list of registered pure components and stock mixtures.

The duration of the operation and the final pressure are specified by the user. The amount of gas added is calculated assuming ideal behavior.

Agitate

The primary objective of this model is to account for the time and power required for mixing the contents of a vessel. The agitation time is specified by the user. In terms of power consumption, the user has the option of specifying either the specific power (in kW/m³) or the absolute power (in kW).

This operation checks to make sure that the liquid level in the vessel is between the specified maximum and minimum limits.

Hold

This operation can be used to represent Sample Analysis, Breaks and other operations that simply require some time. It has no impact on equipment contents.

Evacuate

This operation is used to reduce the pressure of a vessel to a specified final value. The final pressure must be lower than the initial. The initial pressure is equal to the final pressure of the previous operation. The duration of the operation is specified by the user.

This operation affects the amount of gases in the freeboard space. The calculation is done assuming ideal gas behavior.

This operation may result in **VOC Emissions** if volatile compounds are present in the vessel.

Gas Sweep

This operation is used to sweep a vessel with a gas. The sweep gas can be selected from the lists of registered pure components or stock mixtures. The gas flowrate and the duration of the operation are specified by the user. The amount of gas consumed is calculated from the sweep flowrate and process time of the operation. Ideal gas behavior is assumed for converting gas volumetric flowrate to mass flowrate.

This operation may result in **VOC Emissions** if volatile compounds are present in the vessel.

Purge / Inert

Purging is used to remove unwanted gases from the freeboard space of a vessel. It is accomplished by applying pressure with an inert gas and then venting to atmosphere or by pulling vacuum and filling with inert gas or a combination of the above. The model of this operation can handle all three modes of operation.

In the case of Pressure purge, it is assumed that the vessel is pressurized from its initial pressure to "High" pressure and then vented to atmospheric pressure. This cycle can be repeated several times (the number is specified by the user).

In the case of Vacuum purge, it is assumed that the vessel is evacuated from its initial pressure to "Low" pressure and then vented to atmospheric pressure.

In the case of Vacuum and Pressure purge, it is assumed that the vessel is evacuated from its initial pressure to "Low" pressure, pressurized to "High" pressure and vented to atmospheric pressure. This cycle can be repeated several times (the number is specified by the user).

The inert gas is selected from the lists of registered pure components or stock mixtures. Its amount is estimated by assuming ideal gas behavior.

This operation may result in **VOC Emissions** if volatile compounds are present in the vessel.

Vent

In this operation, a vessel that is initially under pressure or vacuum is vented to atmosphere (its final pressure becomes equal to atmospheric). If the vessel is initially under vacuum, venting it to atmosphere results in addition of air into the vessel. If it is initially under pressure, then, a certain amount of freeboard gas leaves the vessel.

The material balances are done assuming ideal gas behavior. The duration of the operation is specified by the user.

This operation may result in **VOC Emissions** if volatile compounds are present and the vessel is initially under pressure.

Batch Component Splitting

This operation models material removal from a vessel, tank (or other equipment). The removal is based on user-specified percentage for each component.

Material Balances

The user specifies the removal percentage of each component, and whether the material splitting regards the liquid phase, vapor phase, or the total contents of the equipment. According to the user specifications the specified amounts are removed through the output stream chosen by the user.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Filtration Operations

Cloth Filtration Operation

This filtration operation is utilized in the following unit procedures: Nutsche Filtration, Basket Centrifugation, and Plate and Frame Filtration.

Filtration Material Balances

The material balances are based on the removal percentage of particulate components and the cake dryness. More specifically, the removal percentage of particulate components determines the amount of those components that is retained in the cake. The cake dryness expressed as Loss On Drying (LOD) % or Cake Porosity determines the amount of solvent and soluble components retained in the cake before washing. If a Cake Wash operation is available in the same procedure, the amount and type of washing determines the displacement of solvent and soluble components in the cake with the wash solvent.

Equipment Sizing and Filtration Time Calculation

In design mode of calculation, the filtration time is specified by the user and the filter area is calculated using the following equation:

$$(\text{Filter Area}) = \frac{(\text{Volume of Slurry Processed per Batch})}{(\text{Cycles per Batch}) \times (\text{Average Filtrate Flux}) \times (\text{Filtration Time})}$$

If the calculated filter area exceeds the maximum filter area that the user specifies, the system automatically assumes multiple units of equal size with a total filter area equal to the calculated.

In rating mode, the user specifies the filter area and the number of units and the system calculates either the average filtrate flux (when the filtration time is specified) or the filtration time (when the flux is specified).

The cake thickness is calculated by dividing the cake volume per cycle by the filter area. If the calculated cake thickness exceeds the user-specified maximum cake thickness, the user is warned.

Cake Discharge

Cake discharge can be modeled using a Transfer Out operation in the same procedure.

Power Consumption

To account for any power requirement for agitation, vacuum, etc. the user can provide a value for the specific power requirement in kW per m² of filter area or simply specify the power consumed.

Cake Wash Operation

Filtration cakes are washed to remove impurities remaining in the interstitial space of the cake. The amount and type of washing determines the displacement of solvent and soluble components in the cake with the wash solvent. For displacement washing type, it is assumed that the solvent and soluble components in the cake are displaced in an embolic (plug-flow) fashion. For slurry washing type, it is assumed that the washing solvent is mixed with the cake and then the cake is filtered to its original dryness.

Equipment Sizing and Filtration Time Calculation

In design mode of calculation, the wash time is specified by the user and the filter area is calculated using the following equation:

$$(FilterArea) = \frac{(Volume_of_Wash_Liquid)}{(Cycles_per_Batch) \times (Average_Filtrate_Flux) \times (Filtration_Time)}$$

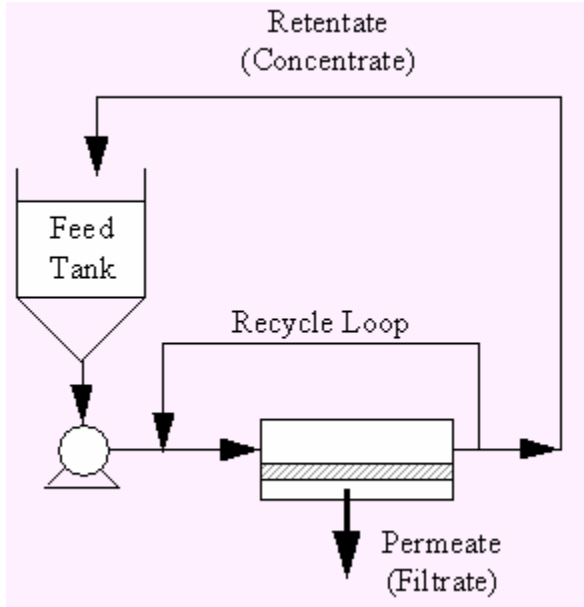
The wash volume is specified on an absolute (L per cycle) or relative basis (L of wash liquid per L of cake).

If the calculated filter area exceeds the maximum filter area that the user specifies, the system automatically assumes multiple units of equal size with a total filter area equal to the calculated.

In rating mode, the user specifies the filter area and the number of units and the system calculates either the average filtrate flux (when the wash time is specified) or the wash time (when the flux is specified).

Membrane Filtration Operation (Batch)

A schematic of batch membrane filtration is shown below. The retentate is returned to the feed tank for recycling through the module. This is the fastest method of concentrating a given amount of material and it requires the minimum membrane area.



Material Balances

In batch concentration, the fraction (F_i) of a component (i) remaining in the retentate at the end of concentration is estimated by the following equation (McGregor, 1986):

$$F_i = (CF)^{R_i-1}$$

where CF is the concentration factor and is given by

$$(CF) = (\text{Feed Volumetric Flowrate}) / (\text{Concentrate Volumetric Flowrate})$$

and R_i is the rejection coefficient of component (i) and is defined by

$$R_i = 1 - (C_{pi} / C_{ci})$$

C_{pi} and C_{ci} are the concentrations of component (i) at the end of filtration in the permeate and concentrate streams, respectively.

To simulate product denaturation due to shear forces during membrane filtration, the user identifies the active and denatured forms of the product component and specifies the denaturation fraction. If the denaturation fraction is zero or if either the active or the denatured product component is not identified, no product denaturation is considered.

Equipment Sizing

In Design Mode, the user specifies the average permeate flux (J), the concentration factor (CF), the Filtration Time, and the rejection coefficients of the various particulate components. Then, the following equation is solved for A (the membrane area):

$$J = V_{\text{feed}} (1 - 1/CF) / A / (\text{Filtration Time})$$

If the calculated membrane area exceeds the maximum allowable membrane area per unit, the system assumes multiple identical units operating in parallel with a total membrane area equal to the calculated. V_{feed} is the volume of material fed to the membrane filtration step per cycle.

The permeate flux depends on the type of the membrane and the composition of the feed stream. For fermentation broths, the flux of microfiltration membranes usually ranges between 10 and 20 L/m²-h. For water treatment with RO membranes, the flux is usually in the range of 22-25 L/m²-h for city water and 13-17 L/m²-h for wastewater. The flux of UF membranes that filter water is 2-3 times the flux of RO membranes. The flux of vibrating membrane filters, such as the VSEP unit from New Logic International, is usually three times the flux of non-vibrating membrane filters.

Filtration Time Estimation

In Rating Mode, the user specifies the area (A) of the membrane filter, the number of identical units operating in parallel, the concentration factor (CF), the rejection coefficients of the various components, and either the Filtration Time or the average permeate flux (J). Then, the following equation is solved either for J (when the filtration time is specified) or for Filtration Time (when the average permeate flux is specified):

$$J = V_{\text{feed}} (1 - 1/\text{CF}) / A / (\text{Filtration Time}) / (\text{Number of microfilters})$$

Equipment Purchase Cost

The equipment purchase cost is estimated using built-in correlations derived from vendor data. It is a function of filter area and filter type (e.g., microfilter, ultrafilter, reverse osmosis). It is also a function of the industry where the unit is used. For instance, the special requirements for piping materials and welding in the biopharmaceutical industries drive the prices up. Consequently, a unit sold to the biopharmaceutical industry may cost 2-5 times the cost of a similar unit (same membrane size) sold to the food or water treatment industries.

For large membrane installations in the food and water industries, the cost of hardware is in the range of \$70-100/m² of membrane area. For small installations in the biopharmaceutical industry, the hardware cost is approximately 10 times higher.

Operating Cost

The cost associated with the periodic replacement of membranes contributes to cost of Consumables. This cost is calculated based on the replacement frequency (in Operating Hours or Number of Cycles), the membrane unit cost (in \$/m²), and the filtration time (specified by the user or calculated by the system).

The membrane unit cost depends on the type of membrane, the size of installation and the type of the industrial end-user. For instance, for large RO installations in the water industry, the unit cost of the membrane is around \$15/m². The cost of UF membranes for similar installations is 3-4 times the cost of RO membranes. For small installations in the biopharmaceutical industry, the unit cost of membranes is in the range of \$150-500/m².

The cost of electricity is estimated based on the Specific Power Requirement (in W/m²) that can be adjusted by the user. The user also has the option to specify the total consumed power. The heating or cooling duty and the associated costs are calculated based on the energy balance around the unit.

Cleaning Requirements

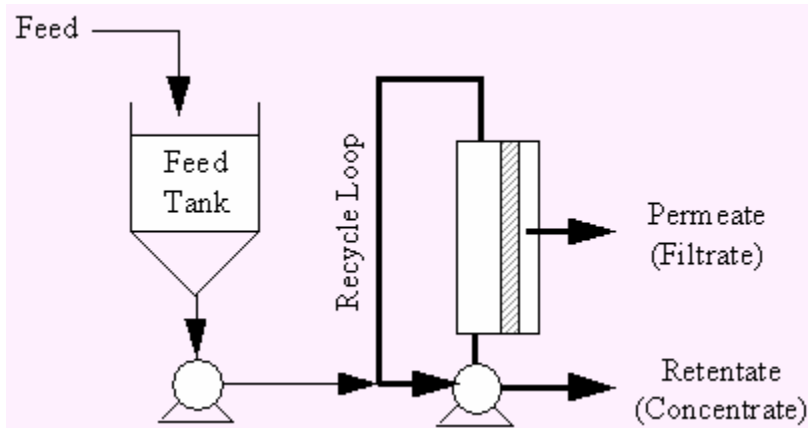
Membrane filters need regular cleaning, every 4 to 30 hours of operation (in biotech applications), in order to maintain high flux and longevity. The average life of membranes strongly depends on the degree of utilization and the operating conditions and in the biotech industry usually ranges from 6 to 12 months (or 1000 to 2000 hours of operation time). In the water industry, membranes are utilized 2-5 years before replacement.

References

1. W.C. McGregor (editor) (1986). *Membrane Separations in Biotechnology*, Marcel Dekker, Inc., New York and Basel.

Membrane Filtration Operation (Continuous)

Continuous membrane filtration (microfiltration, ultrafiltration, reverse osmosis) is employed in plants that require large throughputs (e.g., dairy, beverage, and semiconductor industries). In tangential microfiltration, cross flow parallel to the filter surface is used to enhance filtrate flux. The pore sizes of microfilter membranes usually range from 0.1 to 0.45 microns. Microfiltration is used for solid-liquid separations. In bioprocessing, microfiltration is commonly used for cell harvesting, cell debris removal, and sterilization of cell culture media.



The feed-and-bleed mode of operation comes closest to simulating continuous full-scale operation. The tank shown in the figure above is not really necessary, and this saving in tankage is one advantage of this mode of operation (compared to batch concentration). The disadvantage here is that the process loop is operating continuously at a concentration factor equivalent to the final concentration of a batch system. The flux, therefore, is lower than the average flux in a batch mode, and the membrane area required is correspondingly higher.

To overcome the low flux disadvantage of the "feed-and-bleed" operation, and yet to maintain its continuous nature, large-scale continuous plants are usually staged, using several individual feed-and-bleed stages (to model staged systems in Pro-Designer, multiple membrane filtration units must be used in series). The stages are operated in series as far as concentrate/feed flow is concerned but in parallel with respect to permeate flow. Usually a minimum of 3 stages are required, and 7-10 stages are quite common. The residence time, volume hold-up, and tankage required is much less than for the same duty in batch operation. In addition, such continuous systems can be operated in a sanitary manner over a 24-hour cycle, with a single 2-3 hour cleaning and sanitizing break per 24 hours being adequate. In contrast, due to microbiological or product stability considerations, batch systems are usually restricted to a 4-8 hour operational cycle. Recovering the product, cleaning, sanitizing, and refilling the feed tank make take another 2 hours. The batch plant may be in actual operation for only 2-4 cycles per 24-hour day. Hence although the average flux rate may be higher and membrane area lower with a batch plant, the total volume throughput on a daily basis is higher in the multistage continuous plant.

Material Balances

In feed-and-bleed membrane filtration, the fraction (F_i) of a component (i) remaining in the retentate is estimated by the following equation (McGregor, 1986):

$$F_i = \frac{1}{CF + R_i (1 - CF)}$$

To simulate product denaturation due to shear forces during membrane filtration, the user identifies the active and denatured forms of the product component and specifies the

denaturation fraction. If the denaturation fraction is zero or if either the active or the denatured product component is not identified, no product denaturation is considered.

Equipment Sizing

In Design Mode, the user specifies the average permeate flux (J), the concentration factor (CF), and the rejection coefficients of the various particulate components. Then, the following equation is solved for A (the membrane area):

$$J = V_{\text{feed}} (1 - 1/\text{CF}) / A / (\text{Number of Units})$$

If the calculated membrane area exceeds the maximum allowable membrane area per unit, the system assumes multiple identical units operating in parallel with a total membrane area equal to the calculated. V_{feed} is the volumetric flowrate of the material fed to the filtration step.

In Rating Mode, the user specifies the area (A) of the membrane filter, the number of identical units operating in parallel, the concentration factor (CF), and the rejection coefficients of the various components. Then, the above equation is solved for J to calculate the average permeate flux.

The permeate flux depends on the type of the membrane and the composition of the feed stream. For fermentation broths, the flux of microfiltration membranes usually ranges between 10 and 20 L/m²-h. For water treatment with RO membranes, the flux is usually in the range of 22-25 L/m²-h for city water and 13-17 L/m²-h for wastewater. The flux of UF membranes that filter water is 2-3 times the flux of RO membranes. The flux of vibrating membrane filters, such as the VSEP unit from New Logic International, is usually three times the flux of non-vibrating membrane filters.

Equipment Purchase Cost

The equipment purchase cost is estimated using built-in correlations derived from vendor data. It is a function of filter area and filter type (e.g., microfilter, ultrafilter, reverse osmosis). It is also a function of the industry where the unit is used. For instance, the special requirements for piping materials and welding in the biopharmaceutical industries drive the prices up. Consequently, a unit sold to the biopharmaceutical industry may cost 2-5 times the cost of a similar unit (same membrane size) sold to the food or water treatment industries.

For large membrane installations in the food and water industries, the cost of hardware is in the range of \$70-100/m² of membrane area. For small installations in the biopharmaceutical industry, the hardware cost is approximately 10 times higher.

Operating Cost

The cost associated with the periodic replacement of membranes contributes to cost of Consumables. This cost is calculated based on the replacement frequency (in Operating Hours or Number of Cycles), the membrane unit cost (in \$/m²), and the filtration time (specified by the user or calculated by the system).

The membrane unit cost depends on the type of membrane, the size of installation and the type of the industrial end-user. For instance, for large RO installations in the water industry, the unit cost of the membrane is around \$15/m². The cost of UF membranes for similar installations is 3-4 times the cost of RO membranes. For small installations in the biopharmaceutical industry, the unit cost of membranes is in the range of \$150-500/m².

The cost of electricity is estimated based on the Specific Power Requirement (in W/m²) that can be adjusted by the user. The user also has the option to specify the total consumed power. The heating or cooling duty and the associated costs are calculated based on the energy balance around the unit.

Cleaning Requirements

Membrane filters need regular cleaning, every 4 to 30 hours of operation (in biotech applications), in order to maintain high flux and longevity. The average life of membranes

strongly depends on the degree of utilization and the operating conditions and in the biotech industry usually ranges from 6 to 12 months (or 1000 to 2000 hours of operation time). In the water industry, membranes are utilized 2-5 years before replacement.

References

W.C. McGregor (editor) (1986). *Membrane Separations in Biotechnology*, Marcel Dekker, Inc., New York and Basel.

Diafiltration Operation

In diafiltration, water or some other solvent or buffer is added to the retentate to facilitate the removal of membrane-permeating species along with the water (or other solvent) during filtration. The addition of water (or other solvent) can be conducted under either one of two modes: discontinuous or continuous (O'Sullivan et al., 1984; McGregor, 1986).

In discontinuous operation, permeable solutes are cleared from the retentate by volume reduction (batch concentration), followed by re-dilution with water (or other solvent) and re-concentration in repetitive steps.

In continuous operation, water (or other solvent) is added at the appropriate pH and temperature to the feed tank at the same rate as the permeate flux, thus keeping feed volume constant during processing. Permeable solutes are removed at the same rate as the flux. This mode of diafiltration is particularly useful if the concentration of the retained solute is too high to permit effective discontinuous diafiltration operation for purification.

In the current version of SuperPro Designer, discontinuous operation (batch concentration) can precede and follow a continuous operation (true diafiltration). Any number of batch concentration stages can be specified for each discontinuous operation. In general, if the initial solution is dilute, a concentration step (to reduce the volume of the material) usually precedes a continuous diafiltration step. If the initial solution concentration is rather high, one usually goes directly to continuous diafiltration.

Material Balances

For each batch concentration (discontinuous) operation, when an equal volume reduction takes place in each stage, the final fraction of a component (F_i) remaining in the retentate is estimated as follows:

$$F_i = CF^{n(RC_i - 1)},$$

where CF is the concentration factor in each stage and it is given by

$$(CF) = (\text{Feed Volumetric Flowrate})/(\text{Concentrate Volumetric Flowrate})$$

n is the number of volume reduction stages, and RC_i is the average rejection coefficient of solute (i) defined by

$$R_i = 1 - (C_{pi} / C_{ci})$$

C_{pi} and C_{ci} are the concentrations of component (i) in the permeate and concentrate streams, respectively.

The volume of water (or other solvent) required for dilution is estimated by the following equation:

$$V_{\text{Diluant}} = V_o n \left(1 - \frac{1}{CF}\right),$$

where V_o is the initial feed volume. The value of V_{Diluant} is used to adjust the flowrate of the diluant stream. Consequently, during initialization of a diluant stream (of a diafiltration operation) you only need to specify its composition and not its actual flowrate.

For the continuous operation (true diafiltration), the fraction of a solute remaining in the retentate is estimated by the following equation:

$$F_i = e^{-VPR(1 - RC_i)},$$

where (VPR) is the volumetric permeation ratio, defined as follows:

$$VPR = \frac{\text{Volume of Liquid Permeated}}{\text{Initial Feed Volume}}$$

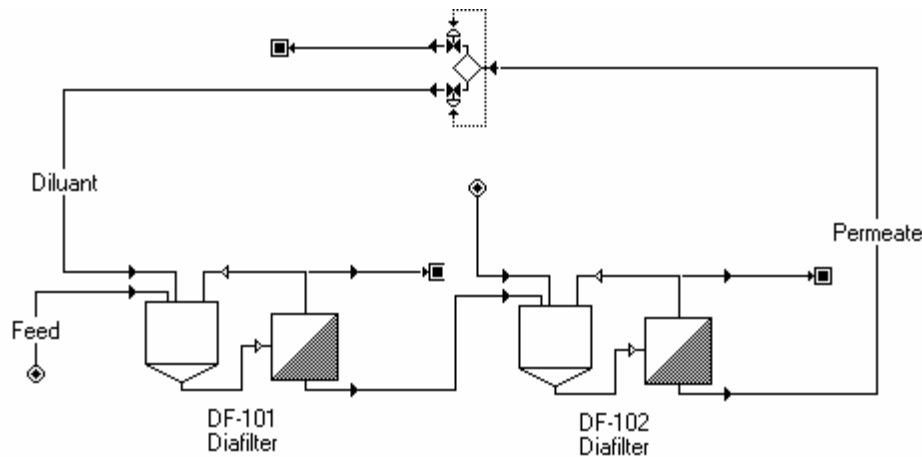
The volume of water (or other solvent) required for dilution is estimated by:

$$V_{\text{Diluant}} = (VPR) (V_0),$$

where V_0 is the initial feed volume. The value of V_{Diluant} is used to adjust the flowrate of the diluant stream as in the case of discontinuous diafiltration.

Case where the diluant stream is not a feed stream. If the diluant stream of a diafilter has a source unit procedure, it must either be associated with a Pull Out operation in that procedure or the procedure must be able to back-propagate flow adjustments in its output stream(s). In the latter case, all input streams of the procedures that back-propagate flow adjustments must be set to "Auto-Adjust" mode (by selecting the appropriate check box on the dialog windows of those input streams).

Case where the diluant stream is part of a recycle loop. If the diluant stream of a diafilter is part of a recycle loop (see figure below), it must be associated with a Pull Out or equivalent operation. Pull Out operations are available in Vessel procedures. The Custom Flow splitter (see figure below) can act as a Pull Out operation if the user selects one of the two bottom splitting specification options (e.g. Preserve Top Flow or Preserve Bottom Flow). For instance, in this case the option "Preserve Bottom Flow" was selected. This allows the diafilter to draw the appropriate amount of diluant. The remainder of the recycled flow (Permeate stream) is directed to the top output stream of the custom flow splitter. If the Diluant flow demand is greater than the Permeate flow, then, the program generates an error message. Recycling of diafiltration buffer is practiced in certain product purification applications, such as blood fractionation.



Operating Cost

The cost associated with the periodic replacement of membranes contributes to cost of Consumables. This cost is calculated based on the replacement frequency (in Operating Hours or Number of Cycles), the membrane unit cost (in \$/m²), and the filtration time (specified by the user or calculated by the system).

The cost of electricity is estimated based on the Specific Power Requirement (in W/m²) that can be adjusted by the user. The heating or cooling duty and the associated costs are calculated based on the energy balance around the unit.

References

1. T. J. O'Sullivan, A. C. Epstein, S. R. Korchin, and N. C. Beaton (1984). Applications of Ultrafiltration in Biotechnology, *CEP* January.
2. W.C. McGregor (editor) (1986). *Membrane Separations in Biotechnology*, Marcel Dekker, Inc., New York and Basel.

Dead End Filtration Operation

Dead-end filtration is usually a polishing step after centrifugation or before a chromatography unit. The filter medium is usually mounted on a cartridge that is replaced periodically.

Material Balances

The material balances are based on the removal percentage of particulate components and the cake dryness (Particle Conc. in Retentate). The removal percentage is either specified by the user or calculated by the system based on the filter medium pore size (0.45 microns by default). The removal percentage of particulate components determines the amount of those components that is retained by the filter. The cake dryness (Particle Conc. in Retentate) expressed in v/v, determines the amount of solvent and soluble components retained in the retentate.

Equipment Sizing and Filtration Time Calculation

In design mode of calculation, the filtration time is specified by the user and the filter area is calculated using the following equation:

$$(\text{Filter Area}) = \frac{(\text{Volume of Slurry Processed per Batch})}{(\text{Cycles per Batch}) \times (\text{Average Filtrate Flux}) \times (\text{Filtration Time})}$$

If the calculated filter area exceeds the maximum that the user specifies, the system automatically assumes multiple units of equal size with a total filter area equal to the calculated.

In rating mode, the user specifies the filter area and the number of units and the system calculates either the average filtrate flux (when the filtration time is specified) or the filtration time (when the flux is specified).

Operating Cost

The cost associated with the periodic replacement of the cartridges contributes to cost of Consumables. This cost is calculated based on the replacement frequency (in Operating Hours or Number of Cycles), the cartridge cost (in \$/cartridge or \$/m² filter area), and the filtration time (specified by the user or calculated by the system).

Rotary Vacuum Filtration Operation

Rotary vacuum filters are used widely in the chemical, biochemical, food, agricultural, and other industries. They feature a horizontal-axis drum covered on the cylindrical portion by filter medium over a grid support structure to allow drainage to manifolds. Sizes (in terms of filter area) range from 0.4 to 95 m² (Perry et al, 1984). Most rotary vacuum filters are fed by operating the drum with about 35% of its circumference submerged in a slurry trough, although submergence can be set for any desired amount between zero and almost total. Common rotation speeds are in the range of 0.1 to 10 RPM. Variable-speed drives are usually provided to allow adjustment for changing cake-formation and drainage rates.

Material Balances

The material balances for the filtration operation are based on the removal percentage of particulate components and the cake dryness. More specifically, the removal percentage of particulate components determines the amount of those components that is retained in the cake. The cake dryness expressed as Loss On Drying (LOD) % or Cake Porosity determines the amount of solvent and soluble components retained in the cake before washing. The amount of washing determines the displacement of solvent and soluble components in the cake with the wash solvent. It is assumed that the solvent and soluble components in the cake are displaced in an embolic (plug-flow) fashion.

Equipment Sizing and Filtration Time Calculation

In design mode of calculation, the filtration time is specified by the user and the filter area is calculated using the following equation:

$$(\text{Filter Area}) = \frac{(\text{Volume of Slurry Processed per Batch})}{(\text{Cycles per Batch}) \times (\text{Average Filtrate Flux}) \times (\text{Filtration Time})}$$

The slurry volume accounts for the feed and the wash water volume. If the calculated filter area exceeds the maximum filter area that the user specifies, the system automatically assumes multiple units of equal size with a total filter area equal to the calculated.

In rating mode, the user specifies the filter area and the number of units and the system calculates either the average filtrate flux (when the filtration time is specified) or the filtration time (when the flux is specified).

References

R.H. Perry, D.W. Green, and J.O. Maloney (1984). *Perry's Chemical Engineers' Handbook*, 6th Edition, McGraw-Hill, New York, p. 19-78.

Air Filtration Operation

This is a very simple operation model that can be used to represent filtration of gaseous streams. In bioprocessing, air filters are used in fermentor air inlet streams to remove dust and prevent contamination. They are also used in gas exhaust streams to prevent release of recombinant and pathogenic microorganisms into the environment.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Equipment Costing

Different functions are available for inlet and exhaust filters that estimate the equipment cost as a function of throughput.

Belt Filtration

Belt filter presses are continuous-feed sludge-dewatering devices that involve the application of chemical conditioning, gravity drainage, and mechanically applied pressure to dewater sludge (Tchobanoglous and Burton, 1991). In most types of belt filter presses, conditioned sludge is first introduced on a gravity drainage section where it is allowed to thicken. In this section, the majority of the free water is removed from the sludge by gravity. Following gravity drainage, pressure is applied in a low-pressure section, where the sludge is squeezed between porous cloth belts. In some units, the low-pressure section is followed by a high-pressure section, where the sludge is subjected to shearing forces as the belts pass through a series of rollers. The squeezing pressure in combination with shear forces induce the release of additional quantities of water from the sludge. The final dewatered sludge cake is removed from the belts by scraper blades.

A typical belt filter press system consists of sludge-feed pumps, polymer-feed equipment, a sludge-conditioning tank (flocculator), a belt filter press, a sludge cake conveyor, and support systems (sludge-feed pumps, washwater pumps, and compressed air).

Belt filter presses are available in metric sizes from 0.5 to 3.5 m in belt width. The most common size used for municipal sludge applications is 2.0 m. Sludge-loading rates vary from 90 to 680 kg/m-h depending on the sludge type and feed concentrations. Hydraulic throughput based on belt width ranges from 1.6 to 6.3 L/m-sec. Note that it is common to express loading rates and sizes of belt filters on the basis of filter width.

Material Balances

The material balances are based on the removal percentage of particulate components and the wt % of solids in cake. The retention of liquid and soluble components is based on the solids content of the cake stream. If the Wash Flow Requirement (in $\text{m}^3/\text{m-h}$) is positive and the wash stream composition is specified, the model adjusts the flowrate of the wash water. The washing is assumed to be of displacement type (embolic displacement of solutes and solvents present in the interstitial space).

Equipment Sizing

In Design Mode, the belt width is calculated by dividing the solids (present in the feed) loading by the specific sludge-loading rate (in kg dry solids/m-h). If the calculated width exceeds the maximum possible (which is specified through the equipment tab), the system assumes multiple units operating in parallel with a total belt width equal to the calculated. In Rating Mode, the user specifies the number of unit and their belt width and the system calculated the sludge-loading rate.

References

1. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", Third edition, Metcalf & Eddy, Inc., McGraw-Hill, p. 864.
2. "Process Design Manual for Sludge Treatment and Disposal", (1979). EPA 625/1-79-011.

Granular Media Filtration

The model used to simulate the behavior of a granular media filter assumes that the bed is composed of one or more layers of packing. Each layer is assumed to have a uniform distribution of particles with a given average (over filtration time and length of that medium's bed depth) binding capacity expressed in mg of solids per cubic centimeter of bed volume (including voids). Based on that binding capacity the effective binding capacity of the whole bed is estimated as the weighted average of each layer, with weight being the percent of total bed depth dedicated to each layer. Furthermore, we assume that the density of the particles used to fill-up each layer of the filter bed is known. To predict a time-dependent variation of the pressure drop across the filter bed as a function of filtration time is beyond the scope of this model. Instead, the model predicts the pressured drop across the clean bed, which sets a lower bound for the pumping requirements to push the feed through. This calculation can be either based on simply a pressure drop rate (possibly measured experimentally) and supplied by the user or by employing one of three different models for predicting the pressure drop rate across a bed packed with particulate material of known properties. The three different models that are available to the user for the estimation of the pressure drop rate across the clean bed and a description of the particulate properties required are presented below:

The Carmen-Kozeny Model:

$$\frac{\Delta P}{L} = \frac{f}{\phi} \frac{1 - \varepsilon}{\varepsilon^3} \frac{\rho u^2}{d}$$

Where,

- ρ is the density of the feed
- u is the linear velocity of the feed
- d is the grain size diameter
- ε is the porosity of the layer
- ϕ is the particle shape factor (1.0 for spheres, 0.82 for rounded sand, 0.75 for average sand, 0.73 for crushed coal and angular sand).
- f is the friction factor, calculated as

$$f = 150 \frac{1 - \varepsilon}{\text{Re}} + 1.75$$

Where, Reynolds Number (Re) is as usual

$$\text{Re} = \frac{\rho u d}{\mu}$$

The Rose Model :

$$\frac{\Delta P}{L} = 1.067 \frac{C_D}{\phi} \frac{1}{\varepsilon^4} \frac{\rho u^2}{d}$$

Where,

ρ is the density of the feed

u is the linear velocity of the feed

d is the grain size diameter

ε is the porosity of the layer

ϕ is the particle shape factor (1.0 for spheres, 0.82 for rounded sand, 0.75 for average sand, 0.73 for crushed coal and angular sand).

C_D is the drag coefficient, calculated as

$$C_D = \frac{24}{Re} + \frac{3}{\sqrt{Re}} + 0.34$$

where, Reynolds Number (Re) is as usual

$$Re = \frac{\rho u d}{\mu}$$

The Fair-Hatch Model:

$$\frac{\Delta P}{L} = k \mu S^2 \frac{(1 - \varepsilon)^2}{\varepsilon^3} \frac{u}{d^2}$$

Where,

- k is a Fair-Hatch filtration constant (must be supplied by the user); k is 5 on sieve openings, 6 when filtration is based on size of separation.
- u is the linear velocity of the feed
- μ is the viscosity of the feed
- d is the grain size diameter
- ε is the porosity of the layer
- S is the particle shape factor (varies between 6.0 for spheres to 8.5 for crushed materials).

Even though some filtration units today can be equipped with a mechanism for continuous backwashing (and this option is available by the simulation model) the majority of filter beds operate in two phases: filtration followed by backwash; therefore they are inherently cyclic. However, most plants operating under continuous conditions will stagger extra units so that the filtration step is performed continuously. The model employed here will automatically estimate all units that are required for a continuous operation (if its mode of operation is set to continuous, which is the default). To estimate the actual washing requirements, the user must either supply a value of washing solvent required per mass of solids withheld or per volume of bed washed. Alternatively, since during the washing stage, the bed is usually fluidized, we could calculate the required washing rate based on the minimum linear velocity that will suspend the bed. The following equation is used to estimate the minimum fluidization velocity:

$$u_o = \frac{d^2 g (\rho_s - \rho) \varepsilon^3}{150 \mu (1 - \varepsilon)}$$

Where,

- μ is the viscosity of the washing solution
- ρ is the density of the washing solution
- ρ_s is the density of the grains
- d is the grain size diameter
- ε is the porosity of the bed
- g is the gravity constant

The above equation is accurate in low Reynolds numbers (below 20) which is usually the case under typical backwashing conditions.

The pressure drop during backwashing is also calculated as :

$$\frac{\Delta P}{L} = (1 - \varepsilon)(\rho_s - \rho)g$$

Where,

- ρ is the density of the washing solution
- ρ_s is the density of the grains
- ε is the porosity of the bed at fluidization conditions
- g is the gravity constant

The above equation is essentially an expression of the fact, that the drag force exerted on the media by the washing fluid is counter balanced by the net force of gravity on the solids.

Equipment Sizing

In Design Mode of calculation we must first understand the role of the overall efficiency percentage. As described in the input data section, the user has to declare which components are likely to be withheld by the filtration step. Then, by default, the model makes the simplifying assumption that the filter's absorbing efficiency with respect to every particulate in the feed is the same and equal to the specified overall efficiency. If this assumption is not adequate, then the user can specify his/her own binding percentages for each component, and then the system will calculate the overall efficiency.

During design mode, typically there is some design constraint that restricts the size of each equipment selected. In this case, the design constraint can be either a maximum allowable pressure drop across the clean bed, or simply a maximum depth.

In summary, a granular media filter set in design mode calculates as follows :

Given

Mode of Operation (Batch/Continuous)

Granular Media Layer Description

Filtration Time

Backwashing Time

Backwash Requirements (set or estimated)
Clean Bed Pressure Drop Rate (set or estimated)
and,
Overall Retention Efficiency
Linear Velocity
Calculate
Number of Units Required
Length of Each Unit
Diameter of Each Unit

In Rating Mode of calculation, the system always calculates the overall efficiency of the filter bed and sets each component's binding % to be the same as the overall filtration efficiency.

In summary, a granular media filter set in rating mode calculates as follows:

Given
Mode of Operation (Batch/Continuous)
Granular Media Layer Description
Filtration Time
Backwashing Time
Backwash Requirements (set or estimated)
Clean Bed Pressure Drop Rate (set or estimated)
and,
Number of Units Required
Length of Each Unit
Diameter of Each Unit
Calculate
Overall Retention Efficiency
Linear Velocity

References

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Baghouse Filtration

In fabric filtration, dusty gas flows into and through a number of filter bags placed in parallel, leaving the dust retained by the fabric. The fabric itself does some filtering of the particles; however, the fabric is more important in its role as a support medium for the layer of dust that quickly accumulates on it. The dust layer is responsible for the highly efficient filtering of small particles for which baghouses are known (this dust layer effect is more important for woven fabrics than for felted fabrics.)

There are many different types of fabrics, different ways of weaving them into various sizes of bags, and different airflow patterns. Extended operation of baghouses requires that the dust be periodically cleaned off the cloth surface and removed from the baghouse. The three common types of baghouses classified by the method used for cleaning the dust from the bags, are (a) reverse-air, (b) shaker and (c) pulse-jet baghouses.

At the center of a baghouse model, is the estimation of the pressure drop across the filter as dust is being accumulated at the bags. The total pressure drop can be viewed as the sum of three terms:

$$\Delta P = \Delta P_f + \Delta P_p + \Delta P_s$$

Where,

ΔP_f is the pressure drop due to the fabric

ΔP_p is the pressure drop due to the particulate layer, and

ΔP_s is the pressure drop due to the baghouse structure.

The last term is usually very low (compared to the other two) and it is neglected, whereas expressions for the other two terms can be acquired by applying Darcy's law for fluid flow through porous media. After substitution of above terms and rearrangement we arrive at the following expression, which is known as the Drag Filter Model for Baghouse Filter Operation:

$$\frac{\Delta P}{u} = \left(\frac{D_f \mu}{K_f} \right) + \left(\frac{\mu}{\rho_\ell K_p} \right) (Lut)$$

Where,

D_f is the depth (in the direction of flow) of the filter (m)

μ is the gaseous viscosity (kg/m-s)

K_f is the permeability of the filter (m²)

K_p is the permeability of the particulate layer (m²)

ρ_ℓ is the bulk density of the particulate layer (kg/m³)

u is the linear velocity of the gas (m/s)

L is the dust loading (kg/m³)

t is the time the bag has been in operation since last cleaning

The above equation is typically expressed in the following form:

$$S = K_e + K_s W$$

Where,

$$S = \frac{\Delta P}{u} \quad \text{Is the Filter Drag (Pa-s/m)}$$

$$K_e = \left(\frac{D_f \mu}{K_f} \right) \quad \text{Is the Extrapolated Clean Cloth Filter Drag (Pa-s/m)}$$

$$K_s = \left(\frac{\mu}{\rho_\ell K_p} \right) \quad \text{Is the "slope" constant for the Filter Drag Model (N-s/kg-m)}$$

$$W = (Lut) \quad \text{Is the areal dust density (kg/m² of fabric)}$$

The above coefficients K_e and K_s are usually measured experimentally from pilot plant tests on dusty gas that is similar to the one for which the design is being made. Since the measurement of K_s is sensitive with respect to the linear velocity range (K_s varies in proportion to the square root of u), if possible, we should adjust the value to account for the difference between the value of linear velocity when K_s was measured and the linear velocity when the model is applied.

All baghouses are constructed with several compartments. When it is time to clean the bags, one compartment is isolated from the dusty gas flow. Then as the bags are being cleaned (either by blowing air in the opposite direction of the flow or by shaking the bags) dust falls into the hopper below the compartment and eventually it is removed. The number of compartments chosen during the design depends on the total flow to be filtered, the maximum allowable (or available) pressure drop, the filtration time (T_f) between two cleanings of the same compartment, and the time required to clean one compartment (T_c).

Equipment Sizing

In Design Mode of calculation the user specifies the desired linear velocity of the gas through the filter and as design constraint the user must specify a maximum allowable number of compartments.

In summary, baghouse filter step in design mode calculates as follows:

Given

Component Retention Coefficients

Filter Drag Model's Coefficients (K_e , K_s) (Set By User or Calculated)

Bag Diameter

Bag Length

Cleaning Time

Either a maximum pressure drop, or a desired filtration time

and,

Linear Velocity

Max Number of Compartments

Number of Bags in Each Compartment

Calculate

Number of Units Required

Number Compartments in Each Unit

In Rating Mode, the user describes the dimensions of a baghouse filter and the model in return calculates the linear velocity of the gas through the filter.

In summary, a baghouse filter step set in rating mode calculates as follows:

Given

Component Retention Coefficients

Filter Drag Model's Coefficients (K_e , K_s) (Set By User or Calculated)

Bag Diameter

Bag Length

Cleaning Time

Either a maximum pressure drop, or a desired filtration time

and,

Number of Units Required

Number Compartments in Each Unit

Number of Bags in Each Compartment

Calculate

Linear Velocity

References

C. David Cooper and F.C. Alley, (1990) *Air Pollution Control : A Design Approach*, McGraw-Hill, Inc.

Electrostatic Precipitation

The process of electrostatic precipitation involves (a) the ionization of contaminated gas (usually air) flowing between electrodes, (b) the charging, migration and collection of contaminants (particles) on oppositely charged plates, and (c) the removal of the particles from the plates. The particles can be either dry dusts or liquid droplets. The air flows through the electrostatic precipitator (ESP) but the particles are left behind on the plates. The material is knocked off or washed off the plates and is collected in the bottom of the ESP. The ESP is unique among air pollution control devices in that the forces of collection act only on the particles and not on the entire air stream. This phenomenon typically results in high collection efficiency with a very low air pressure drop.

We use the Deutsch Equation as the central equation for ESP design. The Deutsch equation relates the collection area with the efficiency of an ESP as follows:

$$\eta = \left(\frac{C_{in} - C_{out}}{C_{in}} \right) = 1 - \exp \left(- \frac{wA}{Q} \right)$$

Where,

- η is the collection efficiency of the ESP
- C_{out} is the concentration of particles in the outlet stream (g/L)
- C_{in} is the concentration of particles in the inlet stream (g/L)
- w is the terminal velocity of the particles under the collection field (m/min)
- A is the overall collection area (m²)
- Q is the volumetric flow of the inlet stream (m³/min)

In case we want to distinguish among several particle ranges, each with a different typical average diameter (and therefore a distinct drifting velocity), the overall efficiency will be a weighted sum of all efficiencies, where the mass fraction of each range is used as the weight in the summation.

The Deutsch equation can be derived by considering the continuity equation for particles flowing between two collection plates, in one collection section, separated by a given distance, and taking into account the fact that the only removal mechanism is a particle flux (with velocity equal to the drift velocity) perpendicular to the flow and towards the plates. More precisely, the Deutsch equation relies on the following assumptions:

1. Gases (and particles) move in the direction of the flow (-x) with constant velocity and no longitudinal mixing.
2. The particles are uniformly distributed in the other two directions (-y and -z).
3. The charging and collecting fields are constant and uniform; the particles quickly attain terminal velocity w in the y direction.
4. Re-entrainment of collected particles is negligible.

If the user does not set the drifting velocities, they are calculated based on field strength data and the permittivity of the flowing gas and several properties of the particles, as follows:

$$w_i = \frac{18\epsilon\epsilon_o E_{ch} E_{co}}{\rho_p d_{pi} (\epsilon + 2)} \tau_i'$$

Where,

- d_{pi} is the diameter of a particle in the ith range (in m)
- ϵ is the relative dielectric constant of the gas
- ϵ_o is the permittivity of free space (constant; 8.85E-12 C/V-m)
- ρ_p is the density of the particles (in g/L)
- E_{ch} is the strength of the charging field (in V/m)
- E_{co} is the strength of the collecting field (in V/m)
- τ_i' is the slip-corrected, characteristic time the particles (in s)

The characteristic time of a particle with a given diameter is calculated as follows:

$$\tau_i' = \frac{4d_{pi}^2 \rho_p C_{Di}}{3\mu(Re)_i C_i'}$$

Where,

- d_{pi} is the diameter of a particle in the ith range (in m)
- μ is the viscosity of the gaseous phase
- ϵ_o is the permittivity of free space (constant; 8.85E-12 C/V-m)
- ρ_p is the density of the particles (in g/L)
- C_{Di} is the drag coefficient of a particle in the ith range
- C_i' is the slip-correction (Cunningham) factor
- $(Re)_i$ is the Reynolds Number calculated as usual

$$(Re)_i = \frac{\rho u d_{pi}}{\mu}$$

The drag coefficient is estimated from an empirical correlation with Re, and the slip correction factor (Cunningham factor) is calculated from the gas's mean free path and the particle's diameter.

Equipment Sizing

In Design Mode of calculation we must first understand the role of the overall efficiency percentage. As described in the input data section, the user has to declare which components are likely to be removed by the ESP. Then, by default, the model estimates an overall efficiency of solids retention, using particle size data and the Deutsch equation. Then the model makes the assumption that all components withheld by the ESP are evenly distributed in all particle

ranges, and sets the removal efficiency for each component set to be removed, to be equal to the overall efficiency. If this assumption is not adequate, the user can specify his/her own removal percentages for each component, and then the system will calculate the overall efficiency.

During design mode, typically there is some design constraint that restricts the size of each equipment selected. In this case, the design constraint is a maximum limit for the sizing of the collection plates' width and height.

In summary, an electrostatic precipitator step in design mode calculates as follows:

Given

Particle Drift Velocities (Set or calculated)

Aspect Ratio

Number of Sections

Corona Power Consumption Data

Fan Efficiency

Overall Pressure Drop,

and,

Overall Retention Efficiency (Set or calculated)

Linear Velocity

Max Plate Height

Max Plate Width

Calculate

Number of Units Required

Number of Ducts in Each Unit

Plate Separation in Each Unit

Plate Length

Plate Height

In Rating Mode, the component retention coefficients are always calculated by the system and set equal to the (calculated) overall efficiency of the ESP.

In summary, an electrostatic precipitator step set in rating mode calculates as follows:

Given

Particle Drift Velocities (Set or calculated)

Aspect Ratio

Number of Sections

Corona Power Consumption Data

Fan Efficiency

Overall Pressure Drop,

and,

Number of Units Required

Number of Ducts in Each Unit

Plate Separation in Each Unit

Plate Length

Plate Height

Calculate

Overall Retention Efficiency

Linear Velocity

References

C. David Cooper and F.C. Alley, (1990) *Air Pollution Control : A Design Approach*, McGraw-Hill, Inc.

Centrifugation and Cyclone Operations

Centrifugation (Disk-Stack, Bowl, Decanter)

This operation is available in Disk-Stack, Bowl, and Decanter centrifugation procedures.

Centrifugation is a common separation operation in the chemical, biochemical, food, and environmental industries. In bioprocessing, centrifugation (mainly disk-stack) is primarily used for recovering and concentrating biomass (cell harvesting), removing cell debris particles after cell disruption, recovering inclusion bodies, and in general separating suspended solids from a liquid solution. Centrifugation is also used to separate immiscible liquid phases that differ in density (e.g., separate oil droplets from an aqueous phase).

Material Balances and Equipment Sizing

Separation by centrifugation is based on the sedimentation principle. Centrifugal separators have been analyzed successfully by using the Sigma Theory (Ambler, 1952, 1961, 1988; Frampton, 1963; Murkes and Carlson, 1978; Axelson, 1985). According to this analysis, to separate from a dispersion all particles (or droplets) of diameter greater than a limit particle diameter (d_{lim}), the maximum separator capacity (throughput) is given by the following equation:

$$Q = \eta \left[\frac{d_{lim}^2 \Delta \rho g}{18\mu} \right] \left[\frac{2\pi}{3g} \omega^2 N \cot \alpha (r_1^3 - r_2^3) \right],$$

where η is the efficiency of the centrifuge (actual throughput/theoretical throughput), d_{lim} is the equivalent Stokes' diameter of the limit particle, $\Delta \rho$ is the density difference between the solid particles (or liquid droplets) and the liquid, μ is the viscosity of the liquid, ω is the angular speed of the disks, N is the number of disks, α is the angle between the disks and the axis of the centrifuge, r_1 and r_2 are the outer and inner diameter of the disks respectively, and Q is the maximum capacity throughput for complete removal of limit particles. The throughput of a centrifuge is proportional to the density difference between the solids and the liquid and proportional to the square of the limiting particle diameter. Therefore, large and dense particles separate more easily than small and light ones.

The term in the second pair of brackets of the equation has units of square meters and is called the *Sigma Factor*. This factor specifies the size of a centrifuge as the equivalent surface area of a sedimentation tank required to achieve the same separation results as the centrifuge.

The term inside the first brackets of the equation has units of velocity [m/sec] and represents the settling velocity of particles in a gravitational field. If V_{lim} is the settling velocity of the limit particles, then all particles with a settling velocity, V , lower than V_{lim} will be removed in the ratio

$x = \frac{V}{V_{lim}}$, where x is the fraction of the particles with settling velocity V that are removed. All particles with a settling velocity greater than V_{lim} will be fully removed.

The case where $\eta = 1$ would describe performance of a centrifuge based on the Stokes' law. Newtonian rheology, hindered settling, non-laminar flow, etc. result in lower values of η . Experience has shown that the efficiency of disk-stack separators is usually less than 50% with an average value of about 30%.

In Design Mode, the user specifies the design component that should be fully recovered and the model estimates the required size of the centrifuge (its Sigma factor) using the above equation. If the calculated sigma factor exceeds the maximum, the program assumes multiple units operating in parallel with a total sigma factor equal to the calculated. In Rating Mode, the user specifies the Sigma factor of the centrifuge and the model estimates the recovery of each component. To accommodate situations where the calculated results do not satisfactorily match experimental data, the user also has the option to specify the removal percentage of all particulate components. The distribution of solvent and soluble components is determined based on the value of "Particles in Heavy Phase (v/v)" that the user specifies.

Equipment Purchase Cost

To estimate the purchase cost of a disk-stack centrifuge, the system uses a function that represents averaged cost data from two different vendors (Alfa-Laval and Westfalia).

References

1. Ambler, C. M. (1952). The Evaluation of Centrifuge Performance. *Chem. Eng. Progress*, 48, 3, 150-158.
2. Ambler, C. M. (1961). The Fundamentals of Separation, including Sharples 'Sigma value' for Predicting Equipment Performance. *Industrial and Engineering Chemistry*, June, 430-433.
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6. Murkes, J. and C-G. Carlsoon (1978). Mathematical Modeling and Optimization of Centrifugal Separation, *Filtration & Separation*, January, 18-21.

Centritech Centrifugation

The Centritech separation system is a new type of centrifuge, designed to handle animal cells, primarily cell cultures in laboratory and pilot plants. It can be used to concentrate cells and clarify media for purposes such as cell recycling, harvesting, washing, clarification and fractionation. The separation takes place in a presterilized flexible tube. The special design of this unit makes it possible to rotate one end of the flexible tube while the other is standing still, thus avoiding the potential risk of infection of the culture that the need for seals on inlet and outlets represents.

The Centritech centrifuge is available for bench and pilot/small plant scales. The bench and pilot scale units handle throughputs of up to 10 and 100 L/h, respectively.

Material Balances

The material balances are based on the removal percentage of particulate components, and the concentration factor (Feed to Retentate Ratio). More specifically, the removal percentage of particulate components determines the amount of particulate components retained in the concentrate. The concentration factor determines the amount of liquid and soluble components retained in the concentrate.

Equipment Selection and Centrifugation Time Calculation

Design mode of calculation. For continuous operation, the throughput is set equal to the volumetric flowrate of the feed stream. For batch operation, the throughput is given by the following equation:

$$(\text{Throughput}) = \frac{(\text{Volume of Material Processed by the Centrifuge per Batch})}{(\text{Cycles per Batch}) \times (\text{Process Time})}$$

If the calculated throughput is less than 10 L/h, a bench scale unit is selected. If it is greater than 10 L/h but lower than 100 L/h, a pilot scale unit is selected. If it is greater than 100 L/h, then, multiple pilot units are assumed operating in parallel so that the throughput of each unit is less than 100 L/h.

Rating mode of calculation. This mode of calculation is used for simulating existing equipment. For a plant operating in batch mode, the primary objective is to calculate the centrifugation (process) time by solving the above equation with respect to process time. For flexibility, the user also has the option to specify the centrifugation time. In that case, the throughput is calculated using the above equation and if it is greater than the maximum, the user is warned.

Operating Cost Estimation

Built-in values are available for the cost of consumables. The default values that are shown on the i/o dialog window of the Centritech centrifuge apply to the pilot scale unit. The user has the option to modify the unit cost as well as the frequency of replacement.

Centrifugation Mode (Pump / Feed / Valve)

Pump mode. This mode of centrifugation requires separate pumps for feed (push) and discharge (pull) lines. The supernatant line opens during separation and discharge, leading to highest perfusion rate. This mode is preferred for scale-up operation.

Feed mode. A single pump is used for feed and discharge lines. The supernatant line closes during discharge to improve clearance. It leads to highest discharge clearance for high cell mass concentration.

Valve mode. Only one pump is used for the supernatant line. A pinch valve opens and closes feed and discharge lines separately. Recovered and recycled cells avoid exposure to pump shear stress.

In the current implementation of the Centritech centrifuge model, the modes of operation have no impact on the model. The information is provided to facilitate communication between professionals involved in the scale up and operation of such units.

Decanting

Decanters are used to separate liquids where there is a sufficient difference in density between the liquids for the droplets to settle readily. Decanters are essentially tanks which give sufficient residence time for the droplets of the dispersed phase to rise (or settle) to the interface between the phases and coalesce. In an operating decanter there will be three distinct zones or bands: clear heavy liquid: separating dispersed liquid (the dispersion zone); and clear light liquid.

Equipment Sizing

Decanters are normally designed for continuous operation, but the same design principles will apply to batch operated units. A great variety of vessel shapes are used for decanters, but for most applications a cylindrical vessel will be suitable, and will be the cheapest shape.

A rough estimate of the decanter volume required can be made by taking a hold-up time of 5 to 10 min, which is usually sufficient where emulsions are not likely to form (Coulson et. al., 1983). The decanter vessel is sized on the principle that the velocity of the continuous phase must be less than the settling velocity of the droplets of the dispersed phase. Plug flow is assumed and the velocity of the continuous phase is calculated using the area of the interface:

$$u_c = L_c/A_i < u_d$$

where

u_d = settling velocity of the dispersed phase droplets, m/s,

u_c = velocity of the continuous phase, m/s,

L_c = continuous phase volumetric flow rate, m³/s,

A_i = area of the interface, m².

Stokes' law is used to determine the settling velocity of the droplets:

$$u_d = [d^2 g (\rho - \rho_c)] / (18 \mu_c)$$

where

d = droplet diameter, m,

u_d = terminal settling velocity of the dispersed phase droplets with diameter d , m/s,

ρ = density of the dispersed phase, kg/m³,

ρ_c = density of the continuous phase, kg/m³,

μ_c = viscosity of the continuous phase, Ns/m²,

g = gravitational acceleration, 9.81 m/s².

The above equation is used to calculate the settling velocity with an assumed droplet diameter of 150 μ m (the droplet diameter can be adjusted by the user), which is well below the droplet sizes normally found in decanter feeds. If the calculated settling velocity is greater than 4×10^{-3} m/s, then a figure of 4×10^{-3} m/s is used.

References

Coulson, J.M., J.F. Richardson, and R.K. Sinnott (1983). *Chemical Engineering - Design*, Volume 6, Pergamon, pp. 344-348.

Hydrocyclone

Hydrocyclones are used for solid-liquid separations and solids classification for particles with size in the range 4 to 500 μm .

Material Balances

The removal efficiency of particles in the feed stream is either set by the user or calculated by the model based on information on particle size distribution. The fraction of solvent(s) and solutes exiting in the heavy phase is determined by the v/v fraction of Particles in Underflow. The rest of this section describes the equations used for calculating the removal efficiency.

The particle diameter for which the hydrocyclone achieves 50% removal efficiency (d_{50}) is calculated by the empirical equation by Bradley (1960):

$$d_{50} = 4.5 \left[\frac{D_c^3 \mu}{L^{1.2} (r_s - r_L)} \right],$$

Where,

- D_c is the body diameter of the cyclone, in cm
- μ is the viscosity of the liquid phase, in cp
- L is the volumetric feed flow rate, in liter/min
- r_L is the density of the liquid, in g/cm³
- r_s is the density of the solid, in g/cm³

In Design Mode, the above equation is solved for D_c to calculate the body diameter of the cyclone.

The separation efficiency for particles with diameter d is related to the d_{50} diameter by the following formula by Bennett (1936):

$$\eta = 100 \left[1 - \exp \left(- \left(d/d_{50} - 0.115 \right)^3 \right) \right].$$

The rest of the hydrocyclone dimensions are calculated based on the body diameter according to the following typical proportions:

- Diameter of inlet duct is $D_c/7$.
- Overflow diameter is $D_c/5$.
- Underflow diameter is $D_c/10$.
- Length of upper cylindrical body is $D_c/3$.
- Overall length is 5 D_c .

References

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Gas Cyclone

Cyclone collectors are used for the separation and recovery of particulate matter from air or process gases. Their use is recommended for particles with diameters greater than 5 μm .

The removal efficiency for particles in the feed stream is either specified by the user or calculated by the model. The rest of this section describes the algorithm for the calculation of the removal efficiency by the model.

The efficiency for each particle size is calculated based on the model proposed by Leith and Licht (1972):

$$\eta = 100 \left[1 - \exp \left[-2(C \Psi)^{1/(2n+2)} \right] \right]$$

C is a dimensionless design number depending upon the physical shape of the cyclone defined as:

$$C = \frac{8K_c}{K_a K_b},$$

where K_c is the cyclone volume constant, $K_a = a/D$ and $K_b = b/D$.

D is the cyclone body diameter. a and b are the inlet height and width of the cyclone, respectively. Ψ is a dimensionless impaction parameter depending upon the operating conditions:

$$\Psi = \frac{\rho_p d_p^2 u_T (n+1)}{18\mu D},$$

where ρ_p is the particle density, d_p is the particle diameter, μ is the gas viscosity and n is the dimensionless exponent of the vortex law for tangential velocity distribution. U_T is the tangential velocity of the particle defined as:

$$u_T = \frac{Q}{ab},$$

where Q is the volumetric flowrate of the gas through the cyclone.

The overall cyclone removal efficiency is the sum of the products of the removal efficiency for each particle size times the weight fraction of that particle size. The weight fractions for each particle size are defined in the particle size distribution.

All the geometrical design characteristics of the cyclone are related to the body diameter D, based on the optimal proportions proposed by Lapple and Sepherd (1939, 1940) which follow:

- Inlet width, $b = D/4$.
- Gas outlet diameter, $D_e = D/4$.
- Inlet height, $a = D/2$.
- Height of upper cylindrical body, $h = 2D$.
- Outlet length, $S = 5D/8$.

- Overall cyclone height, $H = 4D$.
- Outlet duct diameter for dust, $B = D/4$.

References

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Homogenization Operations

Homogenization (High Pressure)

High-pressure homogenization is used in the food industries to homogenize milk, various creams, and other products. The same equipment, operating under higher-pressure drops, is used in the biochemical industries to disrupt (break-open) microorganisms and release intracellular products. For cell disruption, the cell slurry is pumped through a narrow ring gap at pressures up to 1200 bar (depending on the microorganism and the operating mode). The large pressure drop creates high liquid velocities that cause cavitation and turbulence. The resulting fluid oscillation and high shear forces are the primary causes of cell disruption. The disrupted cells release the intracellular protein but because of the high shear rate a fraction of the protein is denatured. To increase the extent of cell disruption, the broth typically passes several times through the disruption unit. The multiple passes also help reduce the viscosity of the suspension by fragmenting the released nucleic acids.

Cell Disruption Kinetics

Cell disruption is described by an empirical model, which relates the fraction of cells disrupted (R) to the pressure drop (ΔP) across the valve and the number of discrete passes (N) (Hetherington et al., 1971):

$$R = 1 - \exp(-k \Delta P^a N),$$

where a is a constant (cell- and equipment-dependent) and k is a release rate constant (cell-, equipment-, and temperature-dependent). Constant a for most microorganisms is approximately equal to 2.9. The fraction of the released intracellular proteins that are denatured (D) is given by the following equation:

$$D = 1 - \exp(-\phi k \Delta P^a N)$$

The parameter ϕ usually has values between 0.0 and 0.3.

To account for situations where the values of a , k , and ϕ are not known but instead actual experimental data are available, the user has the option to specify the release and denaturation fractions.

The user may specify a reaction stoichiometry for the homogenization step representing the disruption of biomass. If, for instance, the product of fermentation is an intracellular protein that forms inclusion bodies, the homogenization reaction may be:

Biomass \rightarrow Debris + Inclusion Bodies + Other Proteins + Nucleic Acids

with a stoichiometry of

(-100 Biomass) + (20 Debris) + (55 Incl. Bodies) + (15 Other Proteins) + (10 Nucleic Acids)

note that this is a mass stoichiometry and the sum of all coefficients must be equal to zero to have conservation of mass.

Homogenization of Food Products

In this case, simply specify the pressure drop through the valve so that the model can calculate the power requirement. There is no need to specify a reaction stoichiometry since no material transformation takes place.

Energy Balances

The electric power required to pump the fluid through the valve is estimated by the following equation:

$$\text{Power} = m \Delta P / (\eta \rho)$$

where m is the mass flowrate of the fluid through the valve, ρ is the density of the fluid, and η is the overall efficiency of the pumping system. It is assumed that all pumping power eventually dissipates into heat that contributes to the cooling or heating requirement.

References

1. Hetherington, P. .J. et al. (1978). Release of Proteins from Baker's Yeast (*Saccharomyces cerevisiae*) by Disruption in an Industrial Homogenizer, *Trans. Instn. Chem. Engrs*, 49.
2. Kula, Maria-Regina and Horst Schutte (1987). Purification of Proteins and the Disruption of Microbial Cells. *Biotechnology Progress*, March, 3, 1, 31-42.

Bead Mill Homogenization

Bead mills are used in various industries to homogenize fluids and powders. In the biochemical industries they are used to disrupt (break-open) microorganisms and release intracellular products. The mechanism of cell disintegration by bead mill is based on the concussion of glass (or steel) beads on the cell surfaces. A bead mill has a horizontal chamber into which cell suspensions can be fed in either batch or continuous mode. The chamber is filled (up to 80-85% of the chamber volume) with glass beads of a fixed diameter which ranges from 0.1 to 3 mm. A rapidly rotating shaft (2,000 - 6,000 RPM) is located in the center of the chamber and is fitted with disks. The rotation of the disks causes the grinding beads to move in a circular manner in the chamber. The kinetic energy transferred from the beads creates impact and shear forces between the individual beads and between the beads and the microbial cells.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the packing density. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Packing Density})$$

Where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units and the program calculates the residence time.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Cell Disruption Kinetics

The rates of product release and denaturation are described by the following equations:

$$\text{Product Release:} \quad R = 1 - \exp(-k t),$$

$$\text{Product Denaturation:} \quad D = 1 - \exp(-\phi k t),$$

where k is a kinetic constant, t is the average residence time of broth in the chamber (usually around 2 min), and ϕ is the denaturation parameter.

To account for situations where the values of k and ϕ are not known but instead actual experimental data are available, the user also has the option to specify the release and denaturation fractions.

The user may specify a reaction stoichiometry for the bead mill representing the disruption of biomass. If, for instance, the product of fermentation is an intracellular protein that forms inclusion bodies, the cell disruption reaction may be:

Biomass --> Debris + Inclusion Bodies + Other Proteins + Nucleic Acids

with a stoichiometry of

(-100 Biomass) + (20 Debris) + (55 Incl. Bodies) + (15 Other Proteins) + (10 Nucleic Acids)

note that this is a mass stoichiometry and the sum of all coefficients must be equal to zero to have conservation of mass.

Homogenization of Food Products

In this case, simply specify the residence time so that the program can estimate the required vessel volume and power requirement. There is no need to specify a reaction stoichiometry since no material transformation takes place.

Energy Balances

The power requirement is estimated using the following equation which was derived from experimental data for cell disruption of *E. coli* (Goldberg, 1987):

$$\text{Power (kW)} = 10.098 + 0.304 \text{ Vol} - 2.95 \times 10^{-4} \text{ Vol}^2,$$

where Vol [liters] is the holding volume of the bead mill. It is assumed that all pumping power eventually dissipates into heat that contributes to the cooling or heating requirement.

References

1. Goldberg (1987). Personal Communication. GlenMills Inc. 203 Brookdale Street, Maywood, N.J. 07607.

Sedimentation/Flotation Operations

Clarification

The purpose of this unit operation model is to simulate the performance of a clarification basin for removing activated sludge as well as other particulate components.

Material Balances

The material balances are based on the removal % of the particulate components and the particulate concentration in sludge (in mg/liter). The removal percentage of particulate components is either specified by the user or calculated by the program using a simple empirical model described by the following equation (Ibrahim and Atasi, 1989):

$$R = \frac{\alpha C_{in}^n}{OR^m}$$

Where R is the removal percent of suspended solids, C_{in} is the influent suspended solids concentration; OR is the overflow rate; α , n , and m are empirical constants. When the empirical model is used, the user is supposed to identify the particulate components that are removed. Please note that the same removal percentage (calculated by the above equation) is applied to all removable components. If this is not an acceptable assumption, then, you may specify the removal percentage of all particulate components by selecting the "Set By User" option. The particulate concentration in sludge determines the amount of liquid and soluble components that remain in the sludge stream.

Equipment Sizing

In Design Mode of calculation, the user either specifies the overflow rate in m^3/m^2 -day or provides the properties (particle diameter and density) of a limiting particle component. If the overflow rate is specified, then, the sedimentation area (cross sectional area of the basin) is calculated by simply dividing the flowrate of the clarified water by the overflow rate. If the calculated cross sectional area exceeds the maximum, the program assumes multiple units operating in parallel with a total cross sectional area equal to the calculated.

If the properties of a limiting particle component are provided, its sedimentation velocity, V_c , is estimated using a modified version of the Stokes' law (Smith and Harriott, 1993). More specifically, the K term is calculated first.

$$K = d \left(\frac{g\rho(\rho_s - \rho)}{\mu^2} \right)^{1/3}$$

Depending on the value of K, different values are assigned to the b_i and n parameters according to the table below.

K	b_i	n
≤ 3.3	24.0	1.0
> 3.3 and ≤ 43.6	18.5	0.6
> 43.6	0.44	0.0

Then, the sedimentation velocity is calculated using the following equation.

$$V_c = \left(\frac{4gd^{1+n}(\rho_s - \rho)}{3b_l\mu^n\rho^{1-n}} \right)^{\frac{1}{2-n}}$$

Where

g = gravitational constant,
 ρ_s = density of particle,
 ρ = density of liquid,
d = diameter of design particle, and
 μ = viscosity of fluid.

Then, the cross sectional area of the clarification basin, A, is calculated by simply dividing the flowrate of the clarified water, Q, by the sedimentation velocity of the design component.

$$A = \frac{Q}{V_c}$$

For continuous-flow sedimentation, the depth of the basin and the time a unit volume of water is in the basin (detention time) should be such that all particles with the design velocity V_c will settle to the bottom of the tank. The design velocity, detention time, and basin depth are related as follows:

$$V_c = \frac{\text{Depth}}{\text{DetentionTime}}$$

In Rating Mode of calculation, the user specifies the number and size of basins and the system calculates the overflow rate.

This operation may result in **VOC Emissions** if volatile compounds are present in the feed stream.

References

1. Hwang, S. T. 1982. "Toxic Emissions from Land Disposal Facilities," *Environmental Progress*. 1: 46-52.
2. Smith J.C. and Harriott, P. (1993). "Unit Operations of Chemical Engineering", 5th Edition, McGraw-Hill.
3. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", Third edition, Metcalf & Eddy, Inc., McGraw-Hill, Sec. 6-3.
4. Ibrahim A.A. and Atasi K.Z. (1989). "Computerized Operating Program for Plant Operation: COPPO", Detroit Water & Sewerage Department, Applied Technology & Evaluation Section, 9300 W. Jefferson, Detroit, MI 48209, presented at the 62nd Annual Conference of Water Pollution Control Federation in San Francisco, CA, Oct. 15-19, 1989.

IP Clarification

The purpose of this unit operation model is to simulate removal of solid particles and/or oil globules by an inclined plate separator.

Equipment Sizing

In Design Mode of calculation, a unit can be sized to remove particles with a settling velocity greater than the settling velocity of a design (limiting) particle. Alternatively, it can be sized to remove oil globules with a rise velocity greater than the rise velocity of a design (limiting) oil globule component. A third option is to design for removal of solid particles as well as oil globules.

Design for Removal of Solid Particles - If the properties of the limiting particle component are provided, its sedimentation velocity, V_c , is estimated using a modified version of the Stokes' law (Smith and Harriott, 1993). More specifically, the K term is calculated first.

$$K = d \left(\frac{g \rho (\rho_s - \rho)}{\mu^2} \right)^{1/3}$$

Depending on the value of K, different values are assigned to the b_l and n parameters according to the table below.

K	b_l	N
≤ 3.3	24.0	1.0
> 3.3 and ≤ 43.6	18.5	0.6
> 43.6	0.44	0.0

Then, the sedimentation velocity is calculated using the following equation.

$$V_c = \left(\frac{4 g d^{1+n} (\rho_s - \rho)}{3 b_l \mu^n \rho^{1-n}} \right)^{\frac{1}{2-n}}$$

Where

- g = gravitational constant,
- ρ_s = density of particle,
- ρ = density of liquid,
- d = diameter of design particle, and
- μ = viscosity of fluid.

The maximum allowable mean horizontal velocity, V_H , is given by:

$$V_H = \min(15V_c, 3 \text{ fpm or } 0.91 \text{ m/min})$$

The turbulence and short-circuit (overdesign) factor, f, is calculated as a function of the ratio (V_H/V_c) using the following equation, which represents curve-fitting of experimental data (API Publication 421, 1989):

$$f = 0.96168 + 0.035455 (V_H/V_c) - 0.000549 (V_H/V_c)^2$$

The user also has the option to specify the turbulence and short-circuit factor. Then, the horizontal area of the unit is calculated by the following equation:

$$A_H = Q / (V_c \times f)$$

Where Q is the feed volumetric flowrate. If the calculated horizontal area exceeds the maximum (specified through the equipment tab), the system assumes multiple units operating in parallel with a total horizontal area equal to the calculated. The horizontal area of a single plate is given by:

$$(\text{Plate } A_H) = (\text{Plate Width}) \times (\text{Plate Length}) \times \cos(\text{Plate Inclination})$$

and the number of plates per unit is given by:

$$(\text{Number of Plates per Unit}) = A_H / (\text{Plate } A_H)$$

Design for Removal of Oil Globules - In oil separation, the Reynolds number for the rising oil globules is usually less than 0.5 and therefore their rise velocity (u_t) is governed by Stokes' law:

$$u_t = \frac{g D^2 (\rho_w - \rho_o)}{18 \mu}$$

Where

ρ_w = density of water,

ρ_o = density of oil,

μ = viscosity,

g = gravity constant,

D = diameter of oil globules.

The maximum allowable mean horizontal velocity, V_H , is given by:

$$V_H = \min(15u_t, 3 \text{ fpm or } 0.91 \text{ m/min})$$

The rest of the calculations are the same as those for removal of solid particles.

Design for Removal of Solid Particles as well as Oil Globules - In this case, the program calculates the settling velocity of the limiting particle component and the rise velocity of the limiting oil globule component and the sizing is done based on the minimum velocity.

Material Balances

The material balances are based on the removal % of particulate and oil globule components that is specified by the user or calculated by the system. The values of "Oil Concentration in Oil Stream" and "Solids Concentration in Sludge Stream" determine the amount of solvent and solute components that are removed with the oil and sludge streams. The removal % of a particulate component, when not specified by the user, is calculated using the following equation:

$$(\text{Removal } \%) = 100 \times (\text{Particle Settling Velocity}) / (f \times \text{Tank Vertical Velocity})$$

In Design Mode, the Tank Vertical Velocity is equal to the settling or rise velocity that is used to size the unit. In Rating Mode, it is equal to the overflow rate (volumetric throughput divided by horizontal area). The parameter f is the turbulence and short-circuit factor. A similar equation (that utilizes the rise velocity instead of settling velocity) is used to estimate removal of oil globule components.

This operation may result in **VOC Emissions** if volatile compounds are present in the feed stream.

References

1. API Publication 421, (1989). "Monographs on Refinery Environmental Control – Management of Water Discharges – Design and Operation of Oil-Water Separators", American Petroleum Institute, 1220 L. Street Northwest, Washington, D.C. 20005.
2. Smith J.C. and Harriott, P. (1993). "Unit Operations of Chemical Engineering", 5th Edition, McGraw-Hill.

Thickening

The purpose of this unit operation model is to simulate the performance of a clarification and thickening basin.

Material Balances

The material balances are based on the removal percentage of particulate components and the solids concentration in sludge (in mg/L). Note that you should only specify removal % for particulate components. The amount of liquid and soluble components in the sludge stream is determined from the sludge solids concentration.

This operation may result in **VOC Emissions** if volatile compounds are present in the feed stream.

Equipment Sizing

In Design Mode, the user specifies the feed volumetric loading rate in m³/m²-day or selects a solids flux model that utilizes the sludge volume index (SVI). When the feed volumetric loading rate is specified, the sedimentation area (cross sectional area of the basin) is calculated by dividing the feed flowrate by the loading rate. If the calculated surface area exceeds the maximum, the system assumes multiple units in parallel with a total surface area equal to the calculated.

The solids flux models for equipment sizing are based on the limiting solids settling flux theory. In general, solids are transported to the bottom of a thickener by the settling velocity component (gravity flux) and the velocity component due to withdrawal in the underflow (underflow flux). The following empirical equation relates the gravity flux to the solids concentration and the SVI:

$$G_s = X V_o \exp (-kX) \quad \text{eq. 1}$$

Where: G_s = solids gravity flux [kg/m²-h],
 X = suspended solids concentration [kg/m³],
 V_o [m/h] and k [m³/kg] are adjustable parameters that depend on SVI.

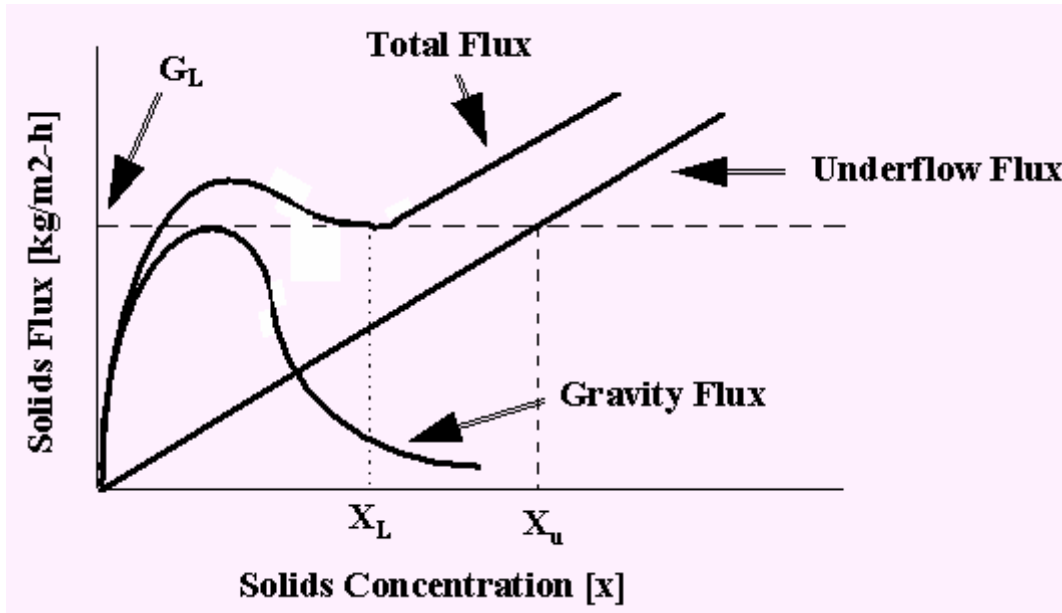
The underflow solids flux is given by the following equation:

$$G_u = X Q_u / A \quad \text{eq. 2}$$

Where: Q_u = underflow volumetric flowrate [m³/h],
 A = Thickener cross sectional area [m],

Consequently, the total flux G_T is:

$$G_T = G_s + G_u = X V_o \exp (-kX) + X Q_u / A \quad \text{eq. 3}$$



The figure above displays the solids gravity flux, underflow flux, and total flux as a function of solids concentration. The limiting solids flux, G_L , which is used to calculate the area of the sedimentation basin corresponds to the minimum value of the total flux. There are two unknowns in eq. 3, the solids concentration X_L that corresponds to G_L and the Q_u/A ratio. Therefore we need two independent equations to solve the problem. Since G_L corresponds to the minimum value of G_T , the first equation which relates X_L with Q_u/A is derived by differentiating G_T with respect to X , setting the derivative equal to zero and solving for Q_u/A :

$$dG_T/dX = V_o \exp(-k X_L) - X_L V_o k \exp(-k X_L) + Q_u/A = 0$$

or ,

$$Q_u/A = X_L V_o k \exp(-k X_L) - V_o \exp(-k X_L) \quad \text{eq. 4}$$

Substituting Q_u/A from eq. 4 into eq. 3, we get G_L as a function of X_L .

$$G_L = (X_L)^2 V_o k \exp(-k X_L) \quad \text{eq. 5}$$

Next we relate X_L with X_u by observing that G_T at X_L is equal to G_u at X_u (see figure above). Therefore:

$$X_L V_o \exp(-k X) + X_L Q_u/A = X_u Q_u/A \quad \text{eq. 6}$$

Substituting Q_u/A from eq. 4 into eq. 6 and eliminating the exponential expressions, which are common in all terms, we get:

$$(X_L)^2 - X_u(X_L) + X_u/k = 0 \quad \text{eq. 7}$$

Eq. 7 is a quadratic equation with respect to X_L and its positive root is given by:

$$X_L = \{ X_u + [(X_u)^2 - 4 X_u/k]^{1/2} \} / 2.0 \quad \text{eq. 8}$$

The user either specifies the parameters V_o and k in the above equations or they are calculated based on the SVI index, which is given as input. Two different models have been implemented for calculating V_o and k as a function of SVI:

Daigger and Roper (1985) developed the first model:

$$V_0 = 7.8 \quad \text{and} \quad k = 0.148 + 0.00210 (\text{SVI})$$

This model was validated for SVI values in the range of 36 to 402 [mL/g].

Wahlberg and Keinath (1988, 1990) developed the second model:

$$V_0 = 15.3 - 0.0615 (\text{SVI}) \quad \text{and}$$

$$k = 0.426 - 0.00384 (\text{SVI}) + 0.0000543 (\text{SVI})^2$$

This model was validated for SVI values in the range of 35 to 220 [mL/g].



Tip

Both of these models were derived for solids concentrations of up to 15 g/liter. Based on our testing, concentrations higher than 12 g/liter lead to very low solids flux and result in excessively high sedimentation areas.

The solids settling flux algorithm in Pro-Designer consists of the following steps:

- 1) V_0 and k , if not specified by the user, are calculated using one of the above models.
- 2) X_L is calculated from eq. 8 as a function of X_u . Note that X_u is the solids concentration in sludge that is specified by the user.
- 3) The limiting solids flux, G_L , is calculated using eq. 3 for $X = X_L$.
- 4) The required area, A , of the sedimentation tank is calculated by dividing the solids mass flowrate in the underflow (based on the removal % of particulate components) by the limiting solids flux, G_L .
- 5) The material balances are completed based on the removal % of particulate components and the specified underflow solids concentration, X_u .

In Rating Mode, the user specifies the number and size of basins and the system calculates the specific feed loading rate. The flux models play no role in rating mode.

References

1. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", Third edition, Metcalf & Eddy, Inc., McGraw-Hill, Sect. 6-5.
2. Daigger, G.T. and R.E. Roper (1985). "The relationship between SVI and activated sludge settling characteristics", *Journal WPCF*, Vol. 57, No. 8, pp. 859-866.
3. Wahlberg, E.J. and T.M. Keinath (1988). "Development of settling flux curves using SVI", *Journal WPCF*, Vol. 60, No. 12, pp. 2095-2100.
4. Keinath, T.M. (1990). "Diagram for designing and operating secondary clarifiers according to the thickening criteria", *Research Journal WPCF*, Vol. 62, No. 3, pp. 254-258.

Flotation

The purpose of this model is to simulate a dissolved-air flotation tank that separates suspended solid or liquid particles from a continuous liquid phase.

Process Description

Separation is brought about by introducing fine gas (usually air) bubbles into the liquid phase. The bubbles attach to the particulate matter, and the buoyant force of the combined particle and gas bubbles is great enough to cause the particle to rise to the surface. Particles that have a higher density than the liquid can thus be made to rise. The rising of particles with lower density than the liquid can also be facilitated (e.g., oil suspension in water).

In dissolved-air flotation systems, air is dissolved in the wastewater under pressure of several atmospheres, followed by release of the pressure to the atmospheric level. In small pressure systems, the entire flow may be pressurized by means of a pump to 4 to 5 atm with compressed air added at the pump suction. The entire flow is held in a retention tank under pressure for several minutes to allow time for the air to dissolve. The pressurized flow is then admitted through a pressure-reducing valve to the flotation tank where the air comes out of solution in minute bubbles throughout the entire volume of liquid. In the larger units, a portion of the dissolved-air flotation effluent (15 to 120 %) is recycled, pressurized, and semi-saturated with air. The recycled flow is mixed with the unpressurized feed stream just before admission to the flotation tank, with the result that the air comes out of solution in contact with particulate matter at the entrance of the tank.

Factors that must be considered in the design of flotation tanks include the concentration of particulate matter, quantity of air used, the particle-rise velocity, and the solids-loading rate. The performance of a dissolved-air flotation system depends primarily on the ratio of the volume of air to the mass of solids (A/S) required to achieve a given degree of clarification. The relationship between the A/S ratio and the solubility of air, the operating pressure, and the concentration of sludge solids for a system in which all the flow is pressurized is given below:

$$\frac{A}{S} = \frac{1.3s_a(fP-1)}{S_a}$$

Where,

$$\frac{A}{S} = \text{air to solid ratio, mL (air)/mg(solids)}$$

$$s_a = \text{air solubility, mL/L}$$

$$f = \text{fraction of air dissolved at pressure P (usually 0.5)}$$

$$P = \text{pressure, atm}$$

$$S_a = \text{sludge solids, mg/L.}$$

For systems without recycle (in other words, with pressurization of the entire feed stream), the above equation is solved for P to calculate the required pressurization level.

The corresponding equation for a system with only pressurized recycle is:

$$\frac{A}{S} = \frac{1.3s_a(fP-1)R}{S_aQ}$$

Where

R = pressurized recycle flowrate, m³/day

Q = mixed-liquor feed flowrate, m³/day.

For systems with recycle, you have the option to specify either the absolute pressure, P, or the recycle flowrate, R, as a percent of the feed flowrate and the above equation is used to calculate R or P, respectively.

Material Balances

The material balances are based on the removal (flotation) % of particulate components and the particulate concentration in sludge (in mg/liter). Note that you should only specify removal % for particulate components. For soluble components, the amount that ends up in the sludge stream depends on the sludge concentration that is specified by the user.

This operation may result in **VOC Emissions** if volatile compounds are present in the feed stream.

Equipment Sizing

In design mode of calculation, the cross sectional area of the flotation tank is calculated by dividing the combined flowrate to the unit, (Q+R), by the surface loading rate, SLR.

$$Area = \frac{Q + R}{LoadingRate}$$

The surface loading rate, SLR, detention time, t_d, and basin depth, d, are related as follows:

$$SLR = \frac{d}{t_d}$$

The above equation is used to calculate the basin depth when the detention time is specified and vice-versa.

In Rating Mode, the user specifies the number and size of basins and the system calculates the surface loading rate.

References

1. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", Third edition, Metcalf & Eddy, Inc., McGraw-Hill, Sect. 6-7.
2. Eckenfelder, W.W. (1989). "Industrial Water Pollution Control", Second edition, McGraw-Hill, Sect. 3-5.

Oil Separation

The purpose of this model is to simulate and design an oil separation tank. In an oil separator, free oil is floated to the surface of a tank and then skimmed off. The conditions holding for the subsidence of particles apply here, except that the lighter-than-water oil globules rise through the liquid. The design of separators as specified by the American Petroleum Institute is based on the removal of all free oil globules larger than 0.015 cm.

Equipment Sizing

In design mode of calculation, the user specifies the rise velocity of the limiting oil globule component or provides the limiting component properties (globule diameter and density) and the viscosity of the water phase. In oil separation, the Reynolds number for the rising oil globules is usually less than 0.5 and therefore their rise velocity (u_t) is governed by Stokes' law:

$$u_t = \frac{gD^2(\rho_w - \rho_o)}{18\mu}$$

Where

ρ_w = density of water,

ρ_o = density of oil,

μ = viscosity,

g = gravity constant,

D = diameter of oil globules.

The minimum cross sectional horizontal area (A_H) is then estimated by the following equation:

$$A_H = F \frac{Q_m}{u_t}$$

Where

Q_m = wastewater flowrate,

$F = F_1 F_2$,

F_1 = factor to compensate for short circuiting (usually equal to 1.2),

F_2 = factor to compensate for turbulence given by the following empirical equation (Eckenfelder, 1989, Table 2-5).

$$F_2 = 0.96168 + 0.035455 \left(\frac{u_H}{u_t} \right) - 0.000549 \left(\frac{u_H}{u_t} \right)^2$$

where u_H is the horizontal velocity and is the minimum of $15 u_t$ and 0.0152 m/s (or 3 fpm).

Then, if the tank depth, d , is specified, the required length, L , of the separator is given by:

$$L = F \frac{u_H}{u_t} d$$

Alternatively, if L is specified, the above equation can be used to calculate d. The minimum vertical cross-sectional area, A_c , is computed from the relationship:

$$A_c = \frac{Q_m}{u_H}$$

In Rating Mode, the user specifies the number and dimensions of the tank(s) and the system calculates the terminal rise velocity.

Material Balances

The material balances are based on the removal % of the suspended components (e.g., oil globules) and the oil concentration in sludge (% v/v). The removal % is either specified by the user or calculated by the system based on the sedimentation theory. Note that you should only specify removal % for suspended components that rise to the surface. For soluble components, the amount that ends up in the oil sludge stream depends on the oil concentration that is specified by the user.

This operation may result in **VOC Emissions** if volatile compounds are present in the feed stream.

References

Eckenfelder, W.W. (1989). "Industrial Water Pollution Control", Second edition, McGraw-Hill, Sect. 3-5.

Chromatography Operations

Column Loading (in a PBA Column)

The main objective of this operation is to estimate the time for loading a column, track recovery yield, and estimate the number and size of columns required (in Desing Mode).

The total binding capacity of the resin refers to all the compounds that bind to the resin. The binding capacity can be estimated experimentally or approximately estimated using Scopes' correlation, providing the molecular weight of the main components is known (Scopes, 1982; p.105, Fig. 5.3).

Column Size Estimation

If Q is the volume of material processed by the column per plant batch time, n is the number of cycles per batch, C_i is the concentration of component i in the feed stream, F_i is the fraction of component i that binds to the resin, then the volume, V, of the column is:

$$V = \frac{Q / n \sum_{i=1}^k C_i F_i}{C} \text{ ODF},$$

where k is the total number of components in the feed stream, ODF is the oversdesign factor, and C is the binding capacity of the resin. When the column length is specified, the diameter is calculated by the following equation:

$$D = \left(\frac{4 V}{\pi L} \right)^{0.5}.$$

If $D > D_{\max}$, then multiple columns are assumed in parallel. Similarly, the user may decide to fix the diameter and have the program calculate the length.

Loading Flowrate Specifications

In terms of loading flowrate you can either specify the linear velocity, the absolute flowrate, or the relative flowrate. These are inter-related:

$$(\text{Absolute Flowrate}) = (\text{Linear Velocity}) \times (\text{Bed Volume}) / (\text{Bed Height})$$

$$(\text{Relative Flowrate}) = (\text{Absolute Flowrate}) / (\text{Bed Volume})$$

Process Time Calculation

The loading is calculated using the following equation:

$$(\text{Loading Time}) = (\text{Bed Height}) \times (\text{Feed Volume}) / (\text{Linear Velocity})$$

The feed volume in the above equation is expressed in "packed bed volumes".

Material Balances

A column may be used to bind either product component(s) or impurity components (specified by the "Resin's Primary Function" buttons on the Loading tab).

In the first case (retention of product components), for a component that binds to the resin its amount in the product stream is equal to its amount in the feed stream times its binding fraction and its elution yield. All components present in the feed stream, that do not bind to resin, exit into the waste stream. Also, all materials in the wash-regeneration-equilibration streams end up in the waste stream. For elution steps, the "Volume in Product Stream" factor which is expressed in "Bed Volumes" determines the fraction of an elution buffer that ends up in the product stream. The remaining exits in the waste stream.

In the case of impurity retention, the fraction of a component that does not bind to the resin ends up in the product stream. For the bound amount, a fraction equal to the elution yield ends up in the product stream. The remaining is sent to the waste stream.

Resin Cost Estimation

The cost associated with resin replacement is estimated as for all consumables. For resins that last several years, the user may decide to depreciate the first resin fill-in by checking the "Is First Resin capitalized" check box in the equipment consumables tab.

References

1. R.K. Scopes (1987). *Protein Purification*, Springer-Verlag.
2. H. Johansson, M. Ostling, G. Sofer, H. Wahlstrom, and D. Low (1988). Chromatographic Equipment for Large-Scale Protein and Peptide Purification. in "Advances in Biotechnological Processes", Vol. 8, Edited by: A. Mizrahi, Published by Alan R. Liss, Inc.
3. R.W. Yost, L.S. Ettre, and R.D. Conlon (1980). *Practical Liquid Chromatography - An Introduction*. ThePerkin-Elmer Corporation.

Column Loading (in a GFL Column)

Gel filtration is primarily used as a polishing step at the end of purification trains. It is also used for buffer exchange following ion exchange steps. In gel filtration the separation media acts as a molecular sieve, separating molecules according to differences in their molecular size and weight. The packed stationary phase consists of numerous porous beads surrounded by a mobile phase. When the sample mixture is applied at the top of the column, large molecules, unable to enter the pores of the beads, pass in between the beads and are eluted first. Smaller molecules with access to the pores are eluted after the larger molecules in order of decreasing size. For globular proteins, elution volumes are directly dependent upon the molecular weight.

Column Size Estimation

In design mode of calculation, the user provides the following information:

- ⇒ Sample volume per injection, B_{SAM} (% of column volume).
- ⇒ Column length (L in m) and maximum column diameter (D_{max} in m) or
- ⇒ Column diameter (D in m) and maximum column length (L_{max} in m).
- ⇒ Linear velocities (u in cm/hr) for loading, elution and washing-stripping-regeneration.
- ⇒ Recovery yield of component i , Y_i .
- ⇒ Overdesign factor, ODF .

If Q is the volume of material processed by the column per plant batch time, n is the number of cycles per batch, then the volume of material fed and processed during one cycle must be equal to one sample volume, that is:

$$\frac{Q}{n} = \frac{B_{SAM}}{100} V \quad \text{or} \quad V = \frac{100 Q}{n B_{SAM}}$$

where V is the column volume. The value of the volume is multiplied by the overdesign factor for conservative design.

If the user decides to specify the length, L , of the column (based on experimental data), the column diameter, D , is calculated by:

$$D = \left(\frac{4 V}{\pi L} \right)^{0.5}.$$

If $D > D_{max}$, then multiple columns are assumed in parallel. Analogous calculation are done when the diameter is fixed and the length is allowed to vary.

sequence even though it has a single output stream. Note that the feed streams to a chromatography column cannot be part of a recycle loop.

Loading Flowrate Specifications

In terms of loading flowrate you can either specify the linear velocity, the absolute flowrate, or the relative flowrate. These are inter-related:

$$(\text{Absolute Flowrate}) = (\text{Linear Velocity}) \times (\text{Bed Volume}) / (\text{Bed Height})$$

$$(\text{Relative Flowrate}) = (\text{Absolute Flowrate}) / (\text{Bed Volume})$$

Process Time Calculation

The loading is calculated using the following equation:

$$(\text{Loading Time}) = (\text{Bed Height}) \times (\text{Feed Volume}) / (\text{Linear Velocity})$$

The feed volume in the above equation is expressed in “packed bed volumes”.

Material Balances

The recovery yield of a component is used to estimate the fraction of that component that ends up in the product stream.

Resin Cost Estimation

The cost associated with resin replacement is estimated as for all consumables. For resins that last several years, the user may decide to depreciate the first resin fill-in by checking the "Is First Resin capitalized" check box in the equipment consumables tab.

References

1. R.K. Scopes (1987). *Protein Purification*, Springer-Verlag.
2. H. Johansson, M. Ostling, G. Sofer, H. Wahlstrom, and D. Low (1988). Chromatographic Equipment for Large-Scale Protein and Peptide Purification. in “Advances in Biotechnological Processes”, Vol. 8, Edited by: A. Mizrahi, Published by Alan R. Liss, Inc.
3. R.W. Yost, L.S. Ettre, and R.D. Conlon (1980). *Practical Liquid Chromatography - An Introduction*. The Perkin-Elmer Corporation.

Column Loading (in a EBA Column)

The main objective of this operation model is to estimate the time for loading a column, track recovery yield, and estimate the number and size of columns required (in Design Mode).

The total binding capacity of the resin refers to all compounds that bind to the resin under actual operating conditions.

Bed Volume Estimation

If V_c is the volume of material processed by the column per cycle, C_i is the concentration of component i in the feed stream, f_i is the fraction of component i that binds to the resin, then the volume, V_b , of the sedimented bed is:

$$V_b = \frac{V_c \sum_{i=1}^k C_i f_i}{C} \text{ODF},$$

Where k is the total number of components in the feed stream, ODF is the overdesign factor, and C is the binding capacity of the resin. The bed height (H_b) is either specified by the user (even in Design Mode) or calculated by the system based on the degree of expansion and other parameters (see below). The bed diameter is calculated using the following equation:

$$D = \left(\frac{4 V_b}{\pi L} \right)^{0.5}.$$

If $D > D_{\max}$, then multiple columns are assumed in parallel. The column diameter is assumed identical to the bed diameter. Analogous calculations are done for columns with a square cross sectional area.

Loading (Process) Time, Residence Time, and Linear Velocity Estimation

The user specifies one of the above three variables and the system calculates the other two. If the bed height (H_b) is specified by the user, we have the following cases:

Fluidization Linear Velocity Specified – In this case, the residence time (t_r) is estimated using the following equation:

$$t_r = \frac{H_b}{U} \quad \text{Eq. (1)}$$

Where U is the fluidization linear velocity. The loading (process) time (t_p) is estimated using the following equation:

$$t_p = t_r \frac{V_c}{V_b} \quad \text{Eq. (2)}$$

Residence Time Specified – In this case, the loading (process) time is estimated using Eq. (2) and Eq. (1) is solved for U to estimate the linear fluidization velocity.

Process Time Specified – In this case, Eq. (2) is solved for t_r to estimate the residence time and Eq. (1) is solved for U to estimate the fluidization linear velocity.

If the user does not specify the bed height, it is estimated based on bed expansion and the expansion safety margin. We have the following cases:

Fluidization Linear Velocity Specified – In this case, the bed height is estimated using the following equation:

$$H_b = \frac{(H_c - \text{Expansion Safety Margin})}{\text{Bed Expansion}} \quad \text{Eq. (3)}$$

The column height, H_c , is always specified by the user. The bed expansion (H/H_o) is either specified by the user (3.0 is the default value) or calculated using the following empirical equation:

$$(\text{Bed Expansion}) = 1 + (A)(\text{Viscosity})(U) \quad \text{Eq. (4)}$$

The multiplier (A) and the liquid viscosity are specified by the user. Then, equations (1) & (2) are used to calculate the loading and residence times.

Residence Time Specified – In this case, the loading time is estimated using Eq. (2). Then, through an iterative algorithm, the program estimates the maximum bed height that does not lead to an overexpansion of the bed. The linear velocity that corresponds to that is estimated using Eq. (1).

Loading Time Specified – In this case, the residence time is estimated using Eq. (2). The rest of the calculations are the same as in the previous case.

Material Balances

For a component that binds to the resin its amount in the product stream is equal to its amount in the feed stream times its binding fraction and its elution yield. All components present in the feed stream, which do not bind to resin, exit into the waste stream. Also, all materials in the wash-regeneration-equilibration streams end up in the waste stream. For elution operations, the "Volume in Product Stream" factor which is expressed in "Sedimented Bed Volumes" determines the fraction of an elution buffer that ends up in the product stream. The remaining exits in the waste stream.

Resin Cost Estimation

The cost associated with resin replacement is estimated as for all consumables. For resins that last several years, the user may decide to depreciate the first resin fill-in by checking the "Is First Resin capitalized" check box in the equipment consumables tab.

References

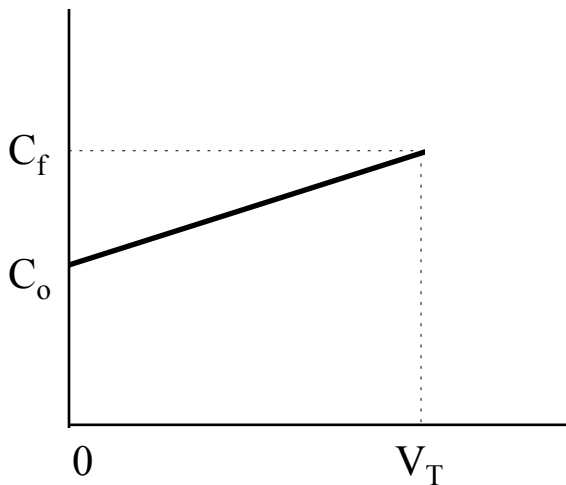
1. Pharmacia Biotech (1997). *Expanded Bed Adsorption – Principles and Methods*, ISBN 91-630-5519-8, Edition AA.
2. Hjorth, R., P. Leijon, A.-K. Barnfield Frej and C. Jagersten (1998). *Expanded Bed Adsorption Chromatography*.

Column Elution

The main objective of this operation is to estimate the elution time and the amount of buffer(s) required.

Buffer Volume Calculation

For isocratic elution, the buffer volume is equal to the bed volume times the volume factor (in packed bed volumes) that is specified by the user. For gradient elution steps, the gradient buffer is generated by mixing two different buffers in continuously varying ratios. This is specified by identifying the two buffer streams (A and B) and providing the initial and final concentration (in mol/liter) of a “key component”. The figure below shows the composition of the key component (varying from C_o to C_f) as a function of the buffer volume. In other words, it is assumed that the concentration varies linearly with buffer volume.



To estimate the volumes of buffer A and B that are mixed to form the gradient elution buffer of volume V_T we do the following simple material balances:

The total number of moles, N , of the key component contained in the gradient buffer of volume V_T is given by:

$$N = V_T (C_o + C_f) / 2 = V_A C_A + V_B C_B$$

where V_A , V_B are the volumes of buffers A and B, respectively, required to form the gradient buffer of volume V_T . C_A and C_B are the concentrations of the key component in buffers A and B, respectively. Also

$$V_T = V_A + V_B$$

The above equations are solved for V_A and V_B and the answer is given below:

$$V_B = V_T [(C_o + C_f)/2 - C_A] / (C_B - C_A) \quad \text{and} \quad V_A = V_T - V_B$$

The calculated buffer volumes are used to adjust the flowrates of the corresponding streams. If the streams have source unit procedures (e.g., buffer preparation tanks), the flowrate

adjustment is recursively back-propagated till flowsheet feed streams are reached. At least one of the flowsheet feed streams that feed into elution or regeneration-equilibration-wash streams must have non-zero flowrate.

Elution Flowrate Specifications

In terms of elution flowrate you can either specify the linear velocity, the absolute flowrate, or the relative flowrate. These are inter-related:

$$(\text{Absolute Flowrate}) = (\text{Linear Velocity}) \times (\text{Bed Area})$$

$$(\text{Relative Flowrate}) = (\text{Absolute Flowrate}) / (\text{Bed Volume})$$

Process Time Calculation

The elution time is calculated using the following equation:

$$(\text{Elution Time}) = (\text{Bed Height}) \times (\text{Buffer Volume}) / (\text{Linear Velocity})$$

The buffer volume in the above equation is expressed in “packed bed volumes”.

Material Balances

A column may be used to bind either product component(s) or impurity components (specified by the “Resin’s Primary Function” buttons on the Loading operation dialog).

In the first case (retention of product components), for a component that binds to the resin its amount in the product stream is equal to its amount in the feed stream times its binding fraction and its elution yield. All components present in the feed stream, that do not bind to resin, exit into the waste stream

The “Volume in Product Stream” factor which is expressed in “Bed Volumes” determines the fraction of an elution buffer that ends up in the product stream. The remaining exits in the waste stream.

In the case of impurity retention, the fraction of a component that does not bind to the resin ends up in the product stream. For the bound amount, a fraction equal to the elution yield ends up in the product stream. The remaining is sent to the waste stream.

Note. Since the flowrate of elution streams is adjusted by the model, the user must make sure that the composition of those streams is correct and not worry about the total stream flowrate.

Column Washing

The main objective of this operation is to estimate the time and buffer required for washing (or equilibrating/rinsing/regenerating) a column.

Buffer Volume Calculation

The buffer volume is equal to the bed volume of the column times the volume factor (in packed bed volumes) that is specified by the user.

Process Time Calculation

The process time is calculated using the following equation:

$$(\text{Process Time}) = (\text{Bed Height}) \times (\text{Buffer Volume}) / (\text{Linear Velocity})$$

The buffer volume in the above equation is expressed in “packed bed volumes”.

Material Balances

All materials used for washing/equilibrating/regenerating a column end up in the waste stream.

Note. Since the flowrate of a wash/equilibration/regeneration stream is adjusted by the model, the user must make sure that the composition of the stream is correct and not worry about the total stream flowrate.

Load (an Ion Exchange Column)

The main objective of this operation is to estimate the time for loading a column (if not specified by the user) and estimate the number and size of columns required (when the equipment is in Desing Mode). The same operation handles loading of cation exchange, anion exchange, and mixed bed columns.

The binding capacity of the resin refers to all the compounds that bind to the resin and whose "Ignore in Sizing?" check-box is not selected. The binding capacity can be specified based on Ion Mass or CaCO₃ hardness.

Column Size Estimation

In Desing mode, the bed volume, V_b , is estimated using the following equation:

$$V_b = (Q)(EBCT)$$

Where Q is the feed volumetric flowrate to the column and EBCT is the empty-bed contact time. The value of EBCT is usually in the range of 1.5 to 7.5 min (Clifford, 1990). In Rating mode, the above equation is used to calculate the value of EBCT.

Dividing the bed volume by the "Bed to Column Height" ratio yields the column volume. When the bed height, H , is specified, its diameter, D , is calculated using the following equation:

$$D = \left(\frac{4 V_b}{\pi H} \right)^{0.5}$$

If $D > D_{max}$, then multiple columns are assumed in parallel. Alternatively, the user may specify the "Bed Height to Diameter" ratio and have the model calculate the bed and column dimensions.

Process (or Breakthrough) Time Calculation

The breakthrough (loading or process) time, t_p , if not specified by the user, is calculated based on the service volume (expressed in bed volumes) or the resin's binding capacity. More specifically, in the case of service volume we use the following equation:

$$t_p = \frac{(\text{Service Volume})(V_b)}{Q}$$

In the case of binding capacity, we use the following equation:

$$t_p = \frac{V_b(N-1)(\text{Resin Binding Capacity})}{(\text{Ion Mass Flow that Binds})}$$

Where N is the number of columns. We consider $(N-1)$ columns because it is assumed that one is always out of service for regeneration. The ion mass flow refers to the fraction of ions that bind to the resin and whose "Ignore in Sizing?" check-box is not selected. If the resin binding capacity is specified based on CaCO₃, then, the ion mass flow refers to equivalent CaCO₃. Please refer to the literature for a straightforward explanation of water hardness expressed on the basis of CaCO₃ (Kemmer, 1988 – Chapter 4).

Resin Cost Estimation

The cost associated with resin replacement is estimated as for all consumables. For resins that last several years, the user may decide to depreciate the first resin fill-in by checking the "Is First Resin capitalized" check box. For water deionization resins, the resin unit cost is around \$1.5/L for cation and around \$4.5/L for anion exchange resins.

Material Balances

The fraction of ions that do not bind to the resin remain in the purified water stream. Those that bind end up in a waste stream during a regeneration operation.

References

1. Clifford, D.A. (1990). Ion Exchange and Inorganic Adsorption. in "Water Quality and Treatment", American Water Works Association, 4th Edition, McGraw-Hill, Inc., Edited by: F. W. Pontius.
2. Kemmer, F.N. (1988). The NALCO Water Handbook, 2nd Edition, McGraw-Hill Book Company.

Column Washing (Ion Exchange Column)

The main objective of this operation is to estimate the time and volume of solution required for washing (or regenerating) a column.

The user has flexibility in specifying any of the following combinations: Duration and Flowrate, Duration and Volume, and Volume and Flowrate. Further, there is considerable flexibility in specifying the flowrate and volume.

Solution Volume Calculation

The (wash/regeneration) solution volume is equal to the bed volume of the column times the volume factor (in packed bed volumes) that is specified by the user. Since the flowrate of a wash /regeneration stream is adjusted by the model, the user must make sure that the composition of the stream is correct and not worry about the total stream flowrate.

Process Time Calculation

When the user specifies the Approach Velocity (also known as Linear Velocity), the process time is calculated using the following equation:

$$(\text{Process Time}) = (\text{Bed Height}) \times (\text{Buffer Volume}) / (\text{Approach Velocity})$$

The buffer volume in the above equation is expressed in “packed bed volumes”.

Material Balances

All materials used for washing/regenerating a column end up in a waste stream.

Adsorption Operations

Load (a GAC Column)

Adsorption of a substance involves its accumulation at the interface between two phases, such as a liquid and a solid (Snoeying, 1990). The molecule that accumulates, or adsorbs, at the interface is called an *adsorbate*, and the solid on which adsorption occurs is the *adsorbent*. Adsorption plays an important role in the purification of water. Activated carbon, for example, can be used to adsorb organic molecules that cause taste and odor, color, mutagenicity, and toxicity.

The main objective of this model is to estimate the time for loading (reaching breakthrough) an activated carbon column (if not specified by the user) and estimate the number and size of columns required (when the equipment is in Design Mode).

Column Size Estimation

In Desing mode, the bed volume, V_b , is estimated using the following equation:

$$V_b = (Q)(EBCT)$$

Where Q is the feed volumetric flowrate to the column and EBCT is the empty-bed contact time. The value of EBCT is usually in the range of 3 to 10 min (Snoeying, 1990). In Rating mode, the above equation is used to calculate the value of EBCT.

Dividing the bed volume by the “Bed to Column Height” ratio yields the column volume. When the bed height, H , is specified, its diameter, D , is calculated using the following equation:

$$D = \left(\frac{4 V_b}{\pi H} \right)^{0.5}$$

If $D > D_{max}$, then multiple columns are assumed in parallel. Alternatively, the user may specify the “Bed Height to Diameter” ratio and have the model calculate the bed and column dimensions.

Process (or Breakthrough) Time Calculation

The breakthrough (loading or process) time, t_p , if not specified by the user, is calculated based on the service volume (expressed in bed volumes) or the adsorbent’s binding capacity. More specifically, in the case of service volume we use the following equation:

$$t_p = \frac{(\text{Service Volume})(V_b)}{Q}$$

In the case of binding capacity, we use the following equation:

$$t_p = \frac{V_b(N-1)(\text{Adsorbent Binding Capacity})}{(\text{Adsorbate Flow that Binds})}$$

Where N is the number of columns. We consider $(N-1)$ columns because it is assumed that one is always out of service for washing/regeneration. The adsorbate flow refers to the fraction of organic compounds that bind to the bed.

Adsorbent Cost Estimation

The cost associated with adsorbent replacement is estimated based on the “Adsorbent Replacement Frequency” and the “Adsorbent Unit Cost” that the user specifies. The unit cost can be specified per unit mass of adsorbent or per canister.

Material Balances

The fraction of adsorbate compounds that do not bind to the bed remain in the purified water stream. Those that bind end up in a waste stream during a washing/regeneration operation.

References

1. Snoeying, V.L. (1990). Adsorption of Organic Compounds. in “Water Quality and Treatment”, American Water Works Association, 4th Edition, McGraw-Hill, Inc., Edited by: F. W. Pontius.
2. Kemmer, F.N. (1988). The NALCO Water Handbook, 2nd Edition, McGraw-Hill Book Company.

Packed Bed (PB) Adsorption

This model is used to simulate the behavior of a packed bed adsorption unit. Gas adsorption is used in industrial applications such as odor control; the recovery of volatile solvents such as benzene, ethanol, trichloroethylene, freon, and so forth; and the drying of process gas streams. The adsorbents used for air pollution control include activated carbon, alumina, bauxite and silica gel. Other special purpose adsorbents include acid-treated clay, aluminosilicate "sieves", Fuller's earth, iron oxide, and magnesia. Activated carbon is by far the most frequently used adsorbent and has virtually displaced all other materials in solvent recovery systems. Generally the capacity of an adsorbent to adsorb a particular adsorbate is directly proportional to the molecular weight and to the vapor pressure of the adsorbate. Typically the capacity of an adsorbent for a specific gas or vapor is represented by an isotherm which is extracted experimentally. There are, however several empirical or semi-empirical correlations that are used to capture adsorption isotherm data. The two most commonly used are Langmuir's and Freundlich's isotherm expressions.

According to Langmuir's mathematical model, the adsorbing capacity q (in mg of adsorbate per g of adsorbent) relates to the adsorbate's concentration C (in mg/L) as follows :

$$q = \frac{K_1 C}{1 + K_2 C}$$

The above equation can actually be derived from first principles and is based on the assumptions that (a) the adsorbed phase is a unimolecular layer, and (b) at equilibrium, the rate of adsorption is equal to the rate of desorption from the surface.

Freundlich's model on the other hand is purely empirical and states that the adsorbing capacity q (in mg of adsorbate per g of adsorbent) relates to the adsorbate's concentration C (in mg/L) as follows :

$$q = KC^{1/n}$$

Either model predicts the adsorption capacity at equilibrium. Under industrial conditions, the bed capacity will seldom exceed 30% or 40% of that indicated by an equilibrium isotherm. Factors to contribute to such a decrease include: the formation of an adsorption zone, loss due to heat wave, loss due to moisture in gas, loss due to residual moisture on adsorbent. Our model takes the adsorption capacity either directly as an input, or estimates the theoretical (equilibrium) capacity using either Langmuir's or Freundlich's equation and a correction factor (to account for practical losses) and the aggregate concentration at the input of all components that are expected to be adsorbed (set by user).

The pressure drop rate across the bed's length can either be supplied by the user or it can be estimated based on Ergun's equation :

$$\frac{\Delta P \varepsilon^3 d}{L(1 - \varepsilon) \rho u^2} = 150 \frac{1 - \varepsilon}{\text{Re}} + 1.75$$

Even though some packed bed adsorption units today can be equipped with a mechanism for continuous regeneration (this option is not available by the simulation model) the majority of adsorption beds operate in two phases: adsorption followed by regeneration; therefore they are inherently cyclic. However, most plants operating under continuous conditions will stagger extra units so that the adsorption step is performed continuously. The model employed here will automatically estimate all units that are required for a continuous operation (if its mode of operation is set to continuous - default -). To estimate the actual fluid requirements for

regeneration (typically steam) the user must either supply a value of regeneration fluid required per mass adsorbed, or per volume of bed regenerated.

Design Mode of Calculation

In this mode of calculation we must first understand the role of the overall efficiency percentage. As described in the input data section, the user has to declare which components are likely to be withheld by the adsorption step. Then, by default, the model makes the simplifying assumption that the filter's absorbing efficiency with respect to every component-to-be-adsorbed in the feed, is the same and equal to the specified overall efficiency. If this assumption is not adequate, then the user can specify his/her own binding percentages for each component, and then the system will calculate the overall efficiency.

During design mode, typically some design constraint restricts the size of each equipment selected. In this case, the design constraint can be either a maximum allowable pressure drop across the bed, or simply a maximum depth.

In summary, a packed bed adsorption filter set in design mode calculates as follows:

Given

- Mode of Operation (Batch/Continuous)
- Adsorbing Capacity (Set or Calculated)
- Breakthrough Time
- Regeneration Time
- Regeneration Solvent Requirements
- Bed Pressure Drop Rate (set or estimated),

and,

- Overall Retention Efficiency
- Linear Velocity

Calculate

- Number of Units Required
- Length of Each Unit
- Diameter of Each Unit

Rating Mode of Calculation

In this mode of calculation, the system always calculates the overall efficiency of the adsorption bed and sets each component's binding % to be the same as the overall adsorption efficiency.

In summary, a packed bed adsorber set in rating mode calculates as follows:

Given

- Mode of Operation (Batch/Continuous)
- Adsorbing Capacity (Set or Calculated)
- Breakthrough Time
- Regeneration Time
- Regeneration Solvent Requirements
- Bed Pressure Drop Rate (set or estimated),

and,

- Number of Units Required
- Length of Each Unit
- Diameter of Each Unit

Calculate

- Overall Retention Efficiency
- Linear Velocity

References

1. C.David Cooper and F.C. Alley, (1990) *Air Pollution Control : A Design Approach*, McGraw-Hill, Inc.
2. D. W. Sundstrom, H. E. Klei, (1980) *Wastewater Treatment*, Prentice Hall, Inc.

Drying Operations

Tray Drying

Tray drying is used for the drying of solids and pastes. Drying is accomplished by direct contact of the wet solid and the drying gas. Tray dryers are useful for small production rates. They operate in batch mode. Due to the labor required for loading and unloading, they are expensive to operate. Frequent applications include drying of valuable products, such as dyes and pharmaceuticals.

Tray dryers consist of a rectangular chamber of sheet metal containing trucks that support racks. Each rack carries a number of shallow trays that are loaded with the material to be dried. Heated air or inert gas is circulated between the trays. Tray dryers may be operated under vacuum, often with indirect heating.

Material and Energy Balances

The material balances are done based on the evaporation percentage of the solvent components. The specific heating requirement along with the amount of solvents that evaporate are used to calculate the total heating requirement. The specific power requirement is used to calculate the overall power requirement. The Drying Gas Requirement along with the amount of solvents that evaporate is used to calculate and adjust the flowrate of the drying gas.

Equipment Sizing

In Design Mode, the user specifies the depth of wet cake and the system calculates the tray area by dividing the calculated wet cake volume by the wet cake depth. If the calculated tray area exceeds the maximum allowable tray area per unit, the system assumes multiple identical units operating in parallel with a total tray area equal to the calculated. In Rating Mode, the user specifies the number of parallel units and their tray area and the system calculates the wet cake depth. If the calculated wet cake depth exceeds the maximum allowable value, the user is warned.

Drying and Cake Discharge Time

The drying time is either specified by the user or calculated based on the evaporation rate (in kg evap./m²-h). The cake discharge time is either specified or calculated based on the discharge rate. The user always specifies the cake discharge set up time. The overall process time is the sum of the drying time, the cake discharge time and the cake discharge set up time.

References

1. Perry R.H. and D.W. Green (1984). *Perry's Chemical Engineers' Handbook*, 6th ed. McGraw-Hill, section 20 pp. 19-22.
2. McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill, 5th ed., pp. 792-793.
3. Coulson J. M. and J. F. Richardson, (1978). *Chemical Engineering*, Vol. 2, Pergamon Press, 3rd ed., pp. 725-727.

Freeze Drying

In freeze dryers, drying is accomplished indirectly under high vacuum and low temperatures (usually below 0 °C). This is done in special vacuum tray dryers. Freeze drying (also known as lyophilization), is frequently used for drying proteins vitamins and other heat sensitive products.

Material and Energy Balances

The material balances are done based on the sublimation percentage of the solvent components. The specific power requirement (based on tray area or sublimation amount) is used to calculate the overall power requirement.

Equipment Sizing

In Design Mode, the user specifies the depth of wet cake and the system calculates the tray area by dividing the calculated wet cake volume by the wet cake depth. The system also calculates the sublimation capacity (in kg H₂O or other solvent per cycle) based on the percentage of components that sublimate. If the calculated sublimation capacity exceeds the maximum, the system assumes multiple units operating in parallel with a total sublimation capacity equal to the calculated. In Rating Mode, the user specifies the number of parallel units, their tray area and their sublimation capacity and the system calculates the wet cake depth. If the calculated wet cake depth exceeds the maximum allowable value, the user is warned.

Drying and Cake Discharge Time

The drying time is either specified by the user or calculated based on the sublimation rate (in mm/h). The cake discharge time is either specified or calculated based on the discharge rate. The user always specifies the cake discharge set up time. The overall process time is the sum of the drying time, the cake discharge time and the cake discharge set up time.

References

1. Geankoplis, C.J. (1983). *Transport Processes and Unit Operations*, Allyn and Bacon, 2nd ed., pp. 554-557.
2. Perry R.H. and D.W. Green (1984). *Perry's Chemical Engineers' Handbook*, 6th ed. McGraw-Hill, section 20 pp. 22-23.

Drying (in a Nutsche Filter)

The material balances for the drying operation are based on the evaporation percentage of volatile components, which are either specified by the user or calculated based on final LOD. If an inert gas is used to facilitate drying, its relative flowrate (kg of gas per kg of solvent evaporated) must be specified by the user. The drying time is either specified by the user or calculated based on the evaporation rate (kg evap./m²-h). The Final Solids temperature simply determines the temperature of the dried cake without having any impact on the energy balance. The heating required for drying is calculated by multiplying the specific heating for drying by the total amount of evaporated solvents. The calculated heating requirement is drawn from the heating agent of choice.

Power Consumption

To account for any power requirement for agitation, vacuum, etc. the user can provide a value for the specific power requirement in kW per m² of filter area or simply specify the power consumed.

Spray Drying

In spray drying, a slurry or liquid solution is dispersed into a stream of hot gas in the form of a mist or fine droplets. Moisture is rapidly vaporized from the droplets, leaving residual particles of dry solid, which are then separated from the gas stream. In a typical spray dryer, the chamber is a cylinder with a short conical bottom.

Material and Energy Balances

The material balances are done based on the evaporation percentage of the solvent component(s). The specific heating (in kg agent /kg of materials that evaporate) is used to calculate the overall heating requirement. The specific power (in kW/(kg/h) feed) is used to calculate the power requirement. The drying gas requirement is used to calculate and adjust the flowrate of the drying gas stream.

Equipment Sizing

In Design Mode, the user specifies the evaporation rate (in kg evap./m³-h) and the system calculates the vessel volume by dividing the vapor mass flowrate by the evaporation rate. The Height/Diameter ratio is used to calculate the height and diameter of the vessel. If the calculated diameter exceeds the maximum, multiple units are assumed that operate in parallel. In Rating Mode, the user specifies the dryer dimensions and the system calculates the evaporation rate.

References

McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill, 5th ed., pp. 801-803.

Fluid Bed Drying

In the fluid-bed dryer, the wet solids are fluidized by the drying gas. Mixing and heat transfer are very rapid. Wet feed is admitted to the top of the bed and dry product is taken out from the side near the bottom. The average time a particle stays in the dryer is typically 30 to 120 sec.

Material and Energy Balances

The material balances are done based on the evaporation percentage of the solvent component(s). The specific heating (in kcal/kg of materials that evaporate) is used to calculate the overall heating requirement. The specific power (in kW/(kg/h) feed) is used to calculate the power requirement. The drying gas requirement is used to calculate and adjust the flowrate of the drying gas stream.

Equipment Sizing

In Design Mode, the average solids velocity and the average solids residence time are used to estimate the required height. Then, the Height/Diameter ratio is used to calculate the vessel diameter. If the calculated diameter exceeds the maximum, multiple units are assumed that operate in parallel. In Rating Mode, the user specifies the dryer dimensions and the average solids velocity and the system calculates the average solids residence time.

References

McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill, 5th ed., pp. 798-800.

Drum Drying

A drum dryer consists of one or more heated metal rolls on the outside of which a thin layer is evaporated to dryness. Dried solid is scraped off the rolls as they slowly revolve. The rolls of a drum dryer are 0.6 to 3 m in diameter. Drum dryers are operated in continuous mode. In some cases, the rolls are covered and the dryer operates under vacuum.

Material and Energy Balances

The material balances are done based on the evaporation percentage of the solvent component(s). The specific heating (in kcal/kg of materials that evaporate) is used to calculate the overall heating requirement. The specific power (in kW/m² drum area) is used to calculate the power requirement.

Equipment Sizing

In Design Mode, the user specifies the evaporation rate (in kg evap./m²-h) and the system calculates the drum area by dividing the vapor mass flowrate by the evaporation rate. If the calculated drum area exceeds the maximum, multiple units are assumed that operate in parallel. In Rating Mode, the user specifies the drum area and the system calculates the evaporation rate.

References

1. McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill, 5th ed., pp. 803-805.
2. Coulson J. M. and J. F. Richardson, (1978). *Chemical Engineering*, Vol. 2, Pergamon Press, 3rd ed., pp. 733-735.

Mix & Dry Operation: Model

Mixing & drying is used for the mixing & drying of solids and pastes in a double cone dryer, cone screw dryer or sphere dryer operating in batch mode. Frequent applications include drying of valuable products in the pharmaceutical, chemical and food industry. The advantage of this operation over the tray drying operation is that the drying, homogenizing and storing steps in a vessel are combined in one method (instead of using a dryer and silo), reducing labor requirement and contamination risks. In addition the simultaneous stirring / agitation can reduce the drying batch time.

Material and Energy Balances

The material balances are done based on the evaporation percentage of the solvent components. The specific heating requirement along with the amount of solvents that evaporate are used to calculate the total heating requirement. The specific power requirement is used to calculate the overall power requirement. The Drying Gas Requirement along with the amount of solvents that evaporate is used to calculate and adjust the flowrate of the drying gas.

Equipment Sizing

The equipment is sized based on its volume. In Design Mode, the user specifies the maximum equipment volume and the maximum allowable working to vessel volume. The user specified Final Solids Bulk Density is used to calculate the dried solids volume (working volume). If calculated volume exceeds the maximum allowable per unit, the system assumes multiple identical units operating in parallel with a total tray area equal to the calculated. In Rating Mode, the user specifies the number of parallel units their volume, and the maximum allowable working to vessel volume. If the calculated working volume exceeds the maximum allowable value, the user is warned.

Drying and Cake Discharge Time

The drying time is either specified by the user or calculated based on the evaporation rate (in kg evap./h).

Rotary Drying

A rotary dryer consists of a revolving cylinder horizontal or slightly inclined toward the outlet. Wet feed enters one end of the cylinder and dry material discharges from the other. The length of the cylinder may range from 4 to more than 10 times its diameter, which may vary from less than 0.3 to more than 3 m. Heating in rotary dryers usually is provided by direct contact of the hot gas with the wet material, but indirect heating (hot gas passing through an external jacket) may also be used.

Material and Energy Balances

The material balances are done based on the evaporation percentage of the solvent component(s). The specific heating (in kcal/kg of materials that evaporate) is used to calculate the overall heating requirement. The specific power (in kW/m² drum area) is used to calculate the power requirement.

Equipment Sizing

In Design Mode, the user specifies the evaporation rate (in kg evap./m³-h) and the system calculates the vessel volume by dividing the vapor mass flowrate by the evaporation rate. The Length/Diameter ratio is used to calculate the length and diameter of the vessel. If the calculated diameter exceeds the maximum, multiple units are assumed that operate in parallel. In Rating Mode, the user specifies the dryer dimensions and the system calculates the evaporation rate.

References

1. Perry R.H. and D.W. Green (1984). *Perry's Chemical Engineers' Handbook*, 6th ed. McGraw-Hill, section 20 pp. 29-33.
2. McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill, 5th ed., pp. 795-798.
3. Coulson J. M. and J. F. Richardson, (1978). *Chemical Engineering*, Vol. 2, Pergamon Press, 3rd ed., pp. 727-733.

Sludge Drying

The purpose of this model is to simulate a generic sludge dryer and perform material and energy balance calculations. The user identifies the volatile components that evaporate and specifies the wt % solids content of the concentrated sludge stream. The same evaporation fraction is assumed for all components that evaporate (this is a reasonable assumption since only water evaporates in the vast majority of sludge dryers). This information is used to calculate the total amount of components that evaporate and estimate the composition of the dried sludge.

The required flowrate of dry air is calculated based on the total amount of solvent(s) that evaporate(s) and the moisture content of entering and exiting air using the following equation:

$$\text{Dry Air Flowrate} = \text{Vapor Mass Flowrate} / (\text{Air Moisture}_{\text{Out}} - \text{Air Moisture}_{\text{In}})$$

The above value of dry air is used to adjust the flowrate of the air stream. The heating requirement is estimated through an energy balance around the unit that considers the sensible heats of the input and output streams as well as the heat of vaporization of water (the most common solvent) and the radiant heat loss. Any heating agent (e.g., steam, natural gas, coal, oil, etc.) can be used/specified to provide the necessary heating requirement.

The Maximum Evaporative Capacity available is used to calculate the number of dryer units that operate in parallel.

References

1. Tchobanoglous G. and F.L. Burton (1991). "Wastewater Engineering: Treatment, Disposal, and Reuse", Third edition, Metcalf & Eddy, Inc., McGraw-Hill, Section 12-14.
2. "Process Design Manual for Sludge Treatment and Disposal", (1979). EPA 625/1-79-011, Chapter 9.
3. Coulson J. M. and J. F. Richardson, (1978). *Chemical Engineering*, Vol. 2, Pergamon Press, 3rd ed., pp. 727-733.

Distillation Operations

Distillation (Continuous)

Distillation is the workhorse separation unit in the petrochemical industries. In the biochemical industries, distillation is used in the recovery and purification of volatile compounds, such as ethanol and organic acids. In the current version of Pro-Designer, a short-cut model is employed to calculate the required number of theoretical stages for a specified separation efficiency.

Material Balances

The user specifies the percentage of each component that ends up in the distillate. Based on this information, the program calculates the overall material balances.

Theoretical Stages

The user identifies the light and heavy keys and provides the relative (to the heavy key component) volatilities (α_i) of the various components. Note that since all relative volatility values are with respect to the heavy key, the heavy key's relative volatility must be 1.0. The minimum reflux ratio (R_{\min}) is estimated using Underwood's (1948) correlation:

$$R_{\min} = \left[\sum_{i=1}^k \frac{\alpha_i X_{Di}}{\alpha_i - \theta} \right] - 1,$$

where k is the number of components, X_{Di} is the mole fraction of component i in the distillate, and θ is determined by trial and error, using the following equation:

$$1 - q = \sum_{i=1}^k \frac{\alpha_i X_{Fi}}{\alpha_i - q},$$

where X_{Fi} is the mole fraction of component i in the feed and q is the quality of the feed:

$$q = \frac{H_{DP} - H_F}{H_{DP} - H_{BP}}$$

- H_{DP} , H_{BP} , and H_F are the enthalpies of the feed as *saturated vapor*, the feed as *saturated liquid*, and the *actual* feed, respectively.

After finding R_{\min} , the program calculates the minimum number of stages (N_{\min}), using the Fenske (1932) equation:

$$N_{\min} = \log \left[\left(\frac{x_l}{x_h} \right)_D \left(\frac{x_h}{x_l} \right)_B \right] \frac{1}{\log \alpha_1},$$

where the subscripts l and h denote the light and heavy key components while D and B denote distillate and bottom.

Equipment Sizing

In Design Mode, the user specifies the desired reflux ratio (R) as a fraction of R_{\min} (R is usually 10-50% greater than R_{\min}) and the program calculates the number of theoretical stages (N) using Gilliland's (1940) correlation as expressed by Eduljee (1975):

$$\frac{N - N_{\min}}{N + 1} = 0.75 - 0.75 \left[\frac{R - R_{\min}}{R + 1} \right]^{0.5668}.$$

The number of actual stages is calculated by dividing the number of theoretical stages by the stage efficiency. The actual number of stages times the stage height yields the height of the column. The column diameter is calculated by dividing the vapor flowrate by the vapor linear velocity that is specified by the user. If the calculated column diameter exceeds the maximum, the program assumes multiple units operating in parallel with a total cross sectional area equal to the calculated.

In Rating Mode, the user specifies the dimensions of the column and the stage efficiency and the program calculates the required reflux ratio.

References

1. Underwood, A.J.V. (1948). *Chem. Eng. Prog.*, **44**, p. 603.
2. Gilliland, E.R. (1940). *Ind. Eng. Chem.*, **32**, p. 1101.

Flash

A flash is a single-stage distillation in which a feed is partially vaporized to give a vapor that is richer in the more volatile components (Henley and Seader, 1981). Computational procedures are available for four different sets of specifications:

- ♦ Operating pressure and temperature: isothermal flash.
- ♦ Operating pressure and zero heat duty: adiabatic flash.
- ♦ Operating pressure and percent of total feed vaporization.
- ♦ Operating pressure and percent vaporization of a specific component in the feed.

Material and Energy Balances

For each component that enters the drum, the following material balance equation holds:

$$Fz_i = Vy_i + Lx_i$$

where F, V, L are the molar flowrates of the feed, vapor and liquid phases respectively and z_i , y_i , x_i are the mole fractions of component i in the three phases.

The mole fractions of component i in the vapor (y_i) and liquid (x_i) phases are related through the partition coefficient

$$K = \frac{y_i}{x_i}$$

Partition coefficients K, are calculated using the vapor and liquid thermodynamic models specified by the user.

The following thermodynamic models are supported for the **vapor phase**:

- ♦ Ideal gas
- ♦ Van der Waals
- ♦ Redlich-Kwong
- ♦ Soave-Redlich-Kwong
- ♦ Peng-Robinson

The following thermodynamic models are supported for the **liquid phase**:

- ♦ Ideal mixture
- ♦ Soave-Redlich-Kwong
- ♦ Peng-Robinson

In the ideal case (i.e. ideal gas and ideal mixture) partition coefficients are independent of composition and are calculated from the vapor pressure correlation (Antoine's equation) for pure components. In all other cases, partition coefficients are composition dependent. In the mixing rules for equations of state (EOS), binary coefficients are assumed to be zero.

The heat duty, Q, for the flash operation is calculated using the overall energy balance:

$$Fh_f + Q = Vh_v + Lh_l$$

where h_f , h_v , h_l are the molar enthalpies of the feed, vapor and liquid streams respectively. For EOS models, excess enthalpy correlations are used. In the adiabatic case ($Q=0$), the energy balance is solved concurrently with the material balances. In all other cases, it is used after the material balances have been solved to calculate the heat duty.

The material and energy balance equations constitute a set of nonlinear algebraic equations which is solved iteratively to calculate the composition of the outlet streams as well as the operating temperature in the cases where the user specifies adiabatic operation or the percent vaporization of total feed or of a specific component in the feed.

Vessel Sizing

In Design Mode, the volume of the drum is calculated by multiplying the outlet liquid phase flowrate by the residence time of the liquid phase in the drum and assuming an optimum height to diameter ratio of 4.0 (Henley and Seader, 1981).

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Equipment Purchase Cost

Equipment purchase cost is based on total vessel volume and material of construction.

References

Henley E. J., and J. D. Seader . (1981). *Equilibrium-Stage Separation Operations in Chemical Engineering*, John Wiley & Sons.

Distillation (Batch)

The batch distillation unit is modeled as a fast, accurate short-cut batch distillation simulation based on the equations of continuous distillation. This method takes advantage of the fact that, at any snapshot in time, the batch distillation column resembles the rectification section of a continuous column. Therefore, the short-cut design methods which have been successfully applied in the simulation of continuous distillation columns are used at every time step in batch distillation. The short-cut method for the simulation of continuous distillation columns used is the Fenske-Underwood-Gilliland (FUG) method. This common empirical method, used to determine reflux and stage requirements of multicomponent continuous distillations, was chosen due to its ease of use and proven applicability.

Vessel Sizing

The pot of the batch distillation unit is sized as a reactor-type of vessel. In design mode of calculation, the working volume is set equal to the volume of material processed per cycle. Dividing the working volume by the initial "Working/Vessel Volume" ratio yields the vessel volume. If the calculated vessel volume excess the max. vessel volume, then multiple units of equal size are assumed with a total volume equal to the calculated vessel volume. In rating mode, the pot volume is specified by the user and the program calculates the initial and final working to vessel volume ratio. If either the initial or the final working/vessel ratio is not between and min and max limits, the user is warned.

Distillation Time

The distillation time can be set by the user or calculated by the model. In the case where the distillation time is calculated by the system, the user must provide the vaporization rate (in kmol/h or L/h) for each operating period. When the distillation time is set by the user, the model reports an average vaporization rate [in kmol/h] for all operating periods.

Material Balances

The relative volatilities of the various components are either specified by the user or calculated by the system assuming ideal solutions and using Antoine's equation for estimating vapor pressures. Non-volatile components (specified by checking the **Non-Volatile?** checkbox) do not participate in vapor-liquid equilibrium calculations and exit the unit through the bottoms stream. If you use the default relative volatility values of one, equal amounts of each volatile component will end up in the distillate stream(s).

Up to five operating periods (or cuts) can be specified. Each cut can represent a desired product or an intermediate fraction. For each operating period, you specify a constant reflux ratio and the mole percentage of the total non-volatile components (that are initially fed into the system) distilled in that period.

The short-cut algorithm consists of an outer loop that steps forward in distillation time and an inner loop that solves the FUG equations at each time step. For the outer loop, the differential balances for total mass in the pot and for each component can be written as follows:

$$\frac{dM}{dt} = \frac{-V}{R+1}$$

where V is the vapor rate and R is the reflux ratio in that operating period

$$\frac{d(Mx_{i,B})}{dt} = x_{i,D} \frac{dM}{dt}$$

The inner loop uses the pot compositions and amount, the vapor rate of the column, the number of stages and the reflux ratio to solve the FUG equations to compute the overhead vapor composition. First, Fenske's equation

$$N_{\min} = \frac{\log\left(\frac{x_{lk,D} x_{hk,B}}{x_{lk,B} x_{hk,D}}\right)}{\log(\alpha_{lk,hk})}$$

is used to compute the minimum number of stages. For batch distillation, the pinch has to occur in the rectifying section of the column. Underwood's equations

$$\frac{(L_{\infty})}{D} = R_{\min} = \frac{\frac{x_{lk,D}}{x_{lk,\infty}} - \alpha_{lk,hk} \frac{x_{hk,D}}{x_{hk,\infty}}}{\alpha_{lk,hk} - 1}$$

are applied to find the pinch point in the rectifying section of the column. Gilliland's equation

$$\frac{N - N_{\min}}{N + 1} = 0.75 \left[1 - \left(\frac{R - R_{\min}}{R + 1} \right)^{0.5668} \right]$$

is used next to relate the minimum number of stages, the minimum reflux ratio, the actual number of stages and the actual reflux ratio. The final equation solved in the inner loop states that the sum of the overhead molar fractions be equal to unity.

The short-cut model works best for simulating columns under the assumptions of constant molar vapor rate during a period and ideal thermodynamics. The assumption being that, at every time step, the liquid and vapor at every stage in the batch column are in equilibrium. The algorithm further assumes that all volatile components distribute to both the distillate and the bottoms, making it a Class 1 separation. If a component is to appear only in the bottom, make sure you specify it as non-volatile.

Energy Balances

The current batch distillation algorithm does not perform energy balances. The condenser and final bottoms temperature that are specified by the user are simply used to set the temperatures of the outlet streams.

Equipment Purchase Cost

The equipment purchase cost includes the cost of the pot vessel as well as the cost of the column and its trays.

Profiles

The batch distillation unit can generate profiles of component concentration (in the receiver, the distillate, and the bottoms) as a function of time. The initialization of recorded data is done through the "Profiles" tab shown below. The user has flexibility in specifying the number of recorded data sets, identifying the streams and components for which compositions are recorded, and selecting the units of recorded variables.

The recorded data sets can be viewed in tabular format by right-clicking on a batch distillation unit and selecting **View Recorded Data as a Table...** (see second figure below). The recorded data sets can be saved in a file in ASCII or Excel (tab-delimited ASCII) format. Then, the

plotting capabilities of Excel (or some other plotting software package) can be used to display the data graphically.

DISTILL-1 (Batch Distillation)

Oper.Cond's | Volumes | Oper.Period | Profiles | Labor, etc. | Description | Scheduling

Number of points: 21

x-Variable: ☒ Time ☐ Progress

y-Variables: ☒ Molar Composition ☐ Concentrations

Component	In Receiver?	In Distillate?	In Bottoms?
Acetalcohol	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Acetone	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Benzene	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Nitrogen	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Oxygen	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Water	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Columnar Reporting Format

Column Width: 12 spaces

Number of Decimals: 4

Space Between Columns: 3 spaces

Units

x-Variable: Distillation Time min

y-Variables

Receiver Comp. %

Distillate Comp. %

Bottoms Comp. %

Labels

x-Variable: Time

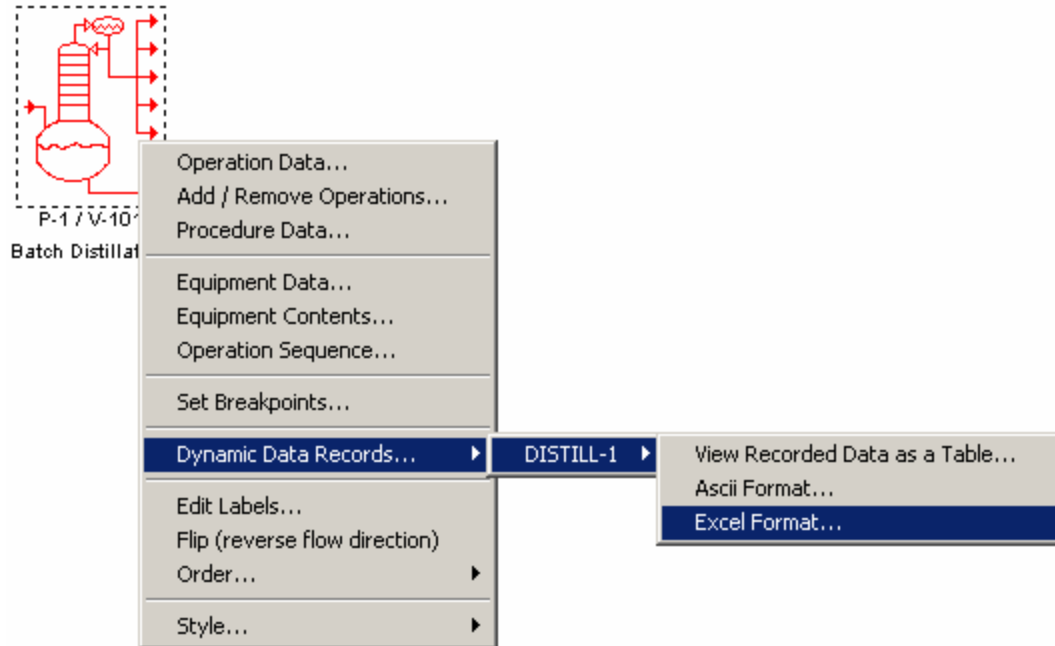
Receiver: %

Distillate: %

Bottoms: %

<< OK OK >> OK Cancel Help

The above dialog window is used to initialize concentration profiles in a batch distillation.



This drop-down menu is displayed when the user right-clicks on a batch distillation. The top line allows user to view the recorded data and the other two to save the recorded data in a formatted file.

References

1. S. Sundaram (1992). *Development of a Fast, Accurate Short-Cut Model for Batch Distillation Simulation*, PhD Thesis, Dept. of Chemical Engineering, MIT, Cambridge, MA.
2. U. M. Diwekar (1995). *BATCH DISTILLATION: Simulation, Optimal Design and Control*, Taylor & Francis Publ., Bristol, PA.

Extraction Operations

Centrifugal Extraction

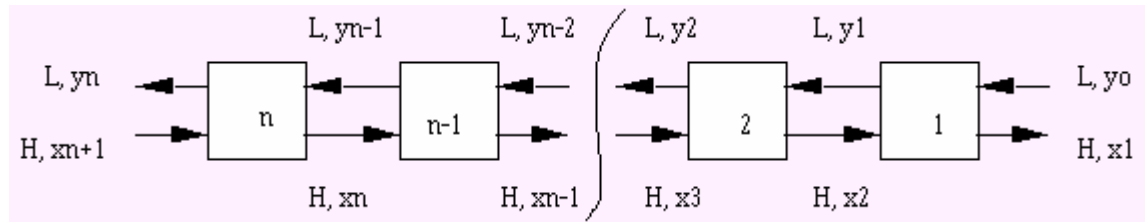
Centrifugal extractors are usually equivalent to a number (2 to 5) of discrete mixer-settler extraction stages. Consequently the technical description of the mixer-settler extraction operation also applies to centrifugal extraction operation. Differences exist in the costing equations.

Mixer-Settler Extraction

The purpose of this model is to simulate extraction in a multi-stage mixer-settler extractor. In the biochemical process industries, extraction is primarily used in the recovery and purification of antibiotics and other low to medium molecular weight products.

Material Balances

The figure below shows a schematic representation of the multiple extraction stages.



L and H are the volumetric flowrates of the light and heavy phase respectively. y_i and x_i is the product composition at stage i in the light and heavy phase respectively. Two streams that exit from a stage are assumed to be at equilibrium. Therefore, $K = \frac{y_i}{x_i}$, where K is the partition coefficient of the product component. The same relation holds for all other components that partition between the light and heavy phase. The generalization of the material balances around each stage yields another equation (Belter, Cussler and Hu, 1988).

$$H x_{n+1} = H \left[\frac{E^{n+1} - 1}{E - 1} \right] x_1 - L y_o,$$

where $E = K L/H$.

In Design Mode, the user specifies the product recovery yield and the above equations are solved for (n) to calculate the required number of extraction stages. In Rating Mode, the user specifies the number of stages and the above equations are solved to calculate the product recovery and the composition of the outlet streams.

Partition coefficients for solvent components should not be provided. To handle limited miscibility, the solubility of each solvent (of the light or heavy phase) in the other solvent should be specified. For single-solvent systems (e.g., aqueous two-phase systems used in biotechnology for the recovery and purification of proteins and other biological molecules), the user in addition specifies the split of the single solvent between the two phases.

Equipment Sizing

In Design Mode, the sizing of the mixer and settler tanks is based on the corresponding residence time that is specified by the user. If the operating throughput exceeds the maximum, the program assumes multiple units operating in parallel with a total throughput equal to the calculated.

References

Belter, P. A., E. L. Cussler, and Wei-Shou Hu (1988). *Bioseparations - Downstream Processing for Biotechnology*, John Wiley & Sons.

Differential Extraction

In differential extractors, solutes are transferred from one phase to the other continuously, but never fast enough to reach equilibrium. The result is significant product isolation, but without the potentially tedious settling times which characterize the staged extractors.

Material Balances

The analysis of the differential extractor depends on three key equations. The first one is the statement of equilibrium:

$$y = K x^*,$$

where x^* is the concentration in the heavy phase which would be in equilibrium with the concentration y in the light phase at a certain position in the column. K is the partition coefficient of the product component between the two phases. The second key equation is a mass balance:

$$Hx + Ly_0 = Hx_0 + Ly,$$

where L and H are the volumetric flowrates of the light and heavy phase respectively. The index 0 denotes the concentration of the product component in the entering streams. The last key equation for the analysis of the differential extractor is:

$$\frac{dx}{dz} = \left(\frac{k_a}{\frac{H}{A}} \right) (x - x^*)$$

where dz is the differential height of the extractor over which the mass transfer takes place, k is the mass transfer coefficient, a is the surface area per unit volume, A is the cross sectional area of the extractor, x is the concentration of the product in the heavy phase and x^* is the concentration of the product component in the heavy phase which would be in equilibrium with the respective light phase concentration y .

Equipment Sizing

In Design Mode, the user specifies the product recovery yield and the above equations are used to calculate the number of transfer units (NTU), and height of a transfer unit (HTU) and consequently the height of the column. The column diameter is calculated by dividing the overall throughput by the flux of combined streams. If the calculated diameter exceeds the maximum, the program assumes multiple units operating in parallel with a total cross sectional area equal to the calculated. In Rating Mode, the user specifies the dimensions of the column and the above equations are used to calculate the product recovery yield and the compositions of the outlet streams.

References

Belter, P. A., E. L. Cussler, and Wei-Shou Hu (1988). *Bioseparations - Downstream Processing for Biotechnology*, John Wiley & Sons.

Phase Change Operations

Condensation

The purpose of this model is to simulate a shell-and-tube surface condenser. Condensation is the process of converting a gas or vapor to liquid. Any gas can be reduced to a liquid by sufficiently lowering its temperature and/or increasing its pressure. The coolant runs in the tube side, while condensation takes place in the shell side. A constant overall heat transfer coefficient is assumed for this model (provided by the user).

Energy Balances

The heat transfer for a surface condenser is governed by the following relationship:

$$Q = U A \Delta T,$$

- Q is the total heat load, kcal / hr.
- U is the overall heat transfer coefficient, kcal / hr -°C - m² .
- ΔT is the mean temperature difference driving force, °C.
- A is the surface area of the condenser, m².

Material Balances

Computational procedures to estimate the condensation efficiency are available for three different sets of specifications for the condenser model:

- ♦ Operating pressure and temperature (isothermal condensation).
- ♦ Operating pressure and percent of total condensation.
- ♦ Operating pressure and percent of condensation of a specific component.

For each component that enters the condenser, the following material balance equation holds:

$$Fz_i = Vy_i + Lx_i ,$$

where F, V, L are the molar flowrates of the feed, vapor and liquid phase respectively and z_i , y_i , x_i are the mole fractions of component i in the three phases.

The mole fractions of component i in the vapor (y_i) and liquid (x_i) phase are related through the partition coefficient K:

$$K = \frac{y_i}{x_i} .$$

Partition coefficients K, are calculated using the vapor and liquid thermodynamic models specified by the user.

The following thermodynamic models are supported for the **vapor phase**:

- ♦ Ideal gas
- ♦ Van der Waals
- ♦ Redlich-Kwong

- ◆ Soave-Redlich-Kwong
- ◆ Peng-Robinson

The following thermodynamic models are supported for the **liquid phase**:

- ◆ Ideal mixture
- ◆ Soave-Redlich-Kwong
- ◆ Peng-Robinson

In the ideal case (i.e. ideal gas and ideal mixture) partition coefficients are independent of composition and are calculated from the vapor pressure correlation (Antoine's equation) for pure components. In all other cases, partition coefficients are composition dependent. In the mixing rules for equations of state (EOS), binary coefficients are assumed to be zero.

The material and energy balance equations constitute a set of nonlinear algebraic equations which is solved iteratively to calculate the composition of the outlet streams as well as the operating temperature in the cases where the user specifies the percent condensation of total feed or of a specific component in the feed.

References

1. Kern D.Q (1965). *Process Heat Transfer*, McGraw-Hill.
2. Henley E. J. and J. D. Seader (1981). *Equilibrium-Stage Separation Operations in Chemical Engineering*, John Wiley & Sons.
3. Theodore L., Buonicore A.J. (1988). *Air Pollution Control Equipment*, 2 (Gases), CRC Press.

Crystallization (Continuous)

This unit operation model simulates crystallization under continuous flow. Crystallization can take place either by addition of a solvent, or by evaporation, or by simple cooling of the solution.

Material Balances

During crystallization, one (or more) components will be converted from their soluble forms into their crystallized forms. Therefore, in order to be able to achieve the desired crystallization effect, you must have defined two distinct components: one to represent the soluble form (e.g., CaSO₄) and one to represent the crystallized form (e.g., CaSO₄-crystal).

The user specifies the crystallization yield of the main soluble product component and identifies its crystallized form. The crystallization yields of all other components that crystallize are specified as a function of the product crystallization yield by a second-degree polynomial equation.

$$(\text{Cryst. Yield of Comp } i) = A + B (\text{Product Yield}) + C (\text{Product Yield})^2.$$

The heat of crystallization and the heat of evaporation should be specified at the reference temperature of 25 °C. If evaporation is considered, it is assumed that it takes place prior to crystallization.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Equipment Purchase Cost

Equipment purchase cost is based on total vessel volume, agitation power and material of construction. It includes the cost of the vessel along with the agitator cost. If the vessel is checked as an "ASME Vessel" (i.e., constructed according to standards published by the American Society of Mechanical Engineers) then it is assumed to withstand pressure to 35 psig and its purchase cost is penalized by 20% over the base vessel cost. If the operating pressure of the vessel is set to a pressure higher than 3 atm, then the vessel's purchase cost is penalized by an 80% increase over the base cost.

Crystallization (Batch)

This operation model simulates batch crystallization in a stirred vessel. Crystallization can take place either by addition of a solvent, or by evaporation, or by simple cooling of the solution.

Material Balances

During crystallization, one(or more) components will be converted from their soluble forms into their crystallized forms. Therefore, in order to be able to achieve the desired crystallization effect, you must have defined two distinct components: one to represent the soluble form (e.g., CaSO_4) and one to represent the crystallized form (e.g., CaSO_4 -crystal).

The user specifies the crystallization yield of the main soluble product component and identifies its crystallized form. The crystallization yields of all other components that crystallize are specified as a function of the product crystallization yield by a second-degree polynomial equation.

The heat of crystallization and the heat of evaporation should be specified at the reference temperature of 25 °C. If evaporation is considered, it is assumed that it takes place prior to crystallization.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Evaporation (Continuous Multi-Effect)

The purpose of this model is to simulate single- or multiple-effect continuous evaporation. The objective of evaporation is to concentrate a solution consisting of a nonvolatile solute and a volatile solvent. In the overwhelming majority of evaporations the solvent is water.

Material Balances

The material balances are based on the evaporation percentage of the various volatile components that is specified by the user.

Energy Balances

The rate of heat transfer Q through the heating surface of an evaporator is the product of three factors: the heat-transfer area A , the overall heat-transfer coefficient U , and the overall temperature drop ΔT , namely:

$$Q = U A \Delta T.$$

The principal measures of the performance of an evaporator are the capacity and the economy. Capacity is defined as the number of kilograms of water (or other solvent) vaporized per hour. Economy is the number of kilograms of water (or other solvent) vaporized per kilogram of steam fed to the unit (McCabe et al., 1993).

Assuming that steam is used for heating, the enthalpy balance for a single effect evaporator has the form:

$$m_S \lambda_S = (m_f - m) H_V - m_f H_f + m H.$$

Where,

- λ_S = latent heat of condensation of steam.
- H_V = specific enthalpy of vapor.
- H_f = specific enthalpy of thin liquor.
- H = specific enthalpy of thick liquor.
- m_S = steam flow rate.
- $m_f - m$ = vapor flow rate.
- m_f = feed liquor flow rate.
- m = thick liquor flow rate.

For solutions having negligible heats of dilution, the enthalpy balances can be calculated from the specific heats and temperatures of the solutions. If the heat of dilution of the liquor being concentrated is appreciable, an enthalpy-concentration diagram has to be used for the values of H_f and H in the above equation.

For a multiple effect evaporator, the heating areas in all the effects are assumed to be equal. This is to obtain economy of construction.

The usual method of feeding a multiple-effect evaporator is to pump the thin liquor into the first effect and send it in turn through the other effects. This is called forward feed. The transfer of the liquid from effect to effect can be done without pumps, since the flow is in the direction of decreasing pressure.

Another common method is backward feed, in which dilute liquid is fed to the last effect and then is pumped through the successive effects to the first. This method requires a pump between each pair of effects.

References

1. McCabe W. L., J. C. Smith ,and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill.
2. Kern D. Q (1965). *Process Heat Transfer*, McGraw-Hill.
3. Coulson J. M. and J. F. Richardson, (1978). *Chemical Engineering*, **2**, Pergamon Press.

Evaporation / Concentration Operation (Batch): Model

This unit operation model simulates batch evaporation in a stirred vessel. Batch evaporation (also known as single-stage batch distillation) is common in the pharmaceutical industries for removing solvents and concentrating solutions.

Material Balances

The user either specifies the evaporation percentage of each volatile component or the extent of concentration in one of the following forms: final liquid volume, evaporation volume, concentration factor, or final concentration of a key component. In the latter case, the evaporation percentage of all volatile components is the same. The volatile components are identified by the user by checking the "Volatile?" check box.

Energy Balances

The heating requirement is calculated based on the Average Heat of Vaporization and the flowrate of the vapor stream. The heating duty for raising the feed streams to the vaporization temperature is also considered.

Evaporation Time

The evaporation time is either specified by the user or calculated by the program based on the evaporation rate. The user always specifies the evaporation setup time.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

References

1. McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill.
2. Kern D. Q (1965). *Process Heat Transfer*, McGraw-Hill.
3. Coulson J. M. and J. F. Richardson, (1978). *Chemical Engineering*, 2, Pergamon Press.

Thin Film Evaporation Operation: Model

Thin film evaporation is a modified falling film evaporation process in which feed enters the top of the jacketed evaporator section and via agitation spreads into a thin turbulent film. The concentrate flows down the bottom outlet of the evaporator and the vapor exits from the top. The user can set the vapor liquid splits or let that be calculated from thermodynamic models. In the later case computational procedures are available for three different sets of specifications:

- Operating pressure and temperature: isothermal evaporation.
- Operating pressure and percent of total feed vaporization.
- Operating pressure and percent vaporization of a specific component in the feed.

In any case, the user can specify whether each component is to be considered as 'volatile' or not.

Material and Energy Balances

For each component that enters the drum, the following material balance equation holds:

$$Fz_i = Vy_i + Lx_i ,$$

where F, V, L are the molar flowrates of the feed, vapor and liquid phase respectively and z_i , y_i , x_i are the mole fractions of component i in the three phases.

The mole fractions of component i in the vapor (y_i) and liquid (x_i) phase are related through the partition coefficient K:

$$K = \frac{y_i}{x_i} .$$

Partition coefficients K, are calculated using the vapor and liquid thermodynamic models specified by the user.

The following thermodynamic models are supported for the **vapor phase**:

- ◆ Ideal gas
- ◆ Van der Waals
- ◆ Redlich-Kwong
- ◆ Soave-Redlich-Kwong
- ◆ Peng-Robinson

The following thermodynamic models are supported for the **liquid phase**:

- ◆ Ideal mixture
- ◆ Soave-Redlich-Kwong
- ◆ Peng-Robinson

In the ideal case (i.e. ideal gas and ideal mixture) partition coefficients are independent of composition and are calculated from the vapor pressure correlation (Antoine's equation) for pure components. In all other cases, partition coefficients are composition dependent. In the mixing rules for equations of state (EOS), binary coefficients are assumed to be zero.

The heat duty, Q , for the evaporation operation is calculated using the overall energy balance:

$$Fh_f + Q = Vh_v + Lh_l$$

where h_f , h_v , h_l are the molar enthalpies of the feed, vapor and liquid streams respectively. For EOS models, excess enthalpy correlations are used. In the adiabatic case ($Q=0$), the energy balance is solved concurrently with the material balances. In all other cases, it is used after the material balances have been solved to calculate the heat duty.

The material and energy balance equations constitute a set of nonlinear algebraic equations which is solved iteratively to calculate the composition of the outlet streams as well as the operating temperature in the case the user specifies the percent vaporization of total feed or of a specific component in the feed.

Equipment Sizing

The sizing variable is the heat transfer area of the evaporator. A constant overall heat transfer coefficient is assumed for this model (provided by the user). In Design mode the heat transfer area is calculated dividing the heat duty by the product of the heat transfer area and the feed temperature difference. In rating mode the user specifies the heat transfer area and the number of units and the equipment capacity utilization is calculated.

Absorption/Stripping Operations

Absorption

In gas absorption, a component from a vapor stream is transferred into a liquid stream with which it comes in contact.

Material Balances

In Design Mode, the material balances are specified by the user (as % Removed) and the separation specifications drive the equipment sizing calculation (see Equipment sizing). In Rating Mode, the removal efficiency (% removed) is either set by the user or calculated by the model. Reactions can take place in the liquid phase, if reactions are present, and the reaction calculations are done after the separation calculations.

Equipment Sizing

In Design Mode, the height Z of the column is calculated from the height of the transfer unit HTU and the number of transfer units NOG :

$$Z = HTU * NOG$$

The number of transfer units is given by:

$$N_{OG} = \frac{A}{A-1} \ln \left(\frac{\frac{y_1 - mx_2}{y_2 - mx_2} (A-1) + 1}{A} \right)$$

- A is the absorption factor defined as L / mG
- L is the volumetric flow rate of the liquid stream.
- G is the volumetric flow rate of the gas stream.
- m is the slope of the equilibrium curve (equal to the Henry's law constant for dilute solutions).
- y_1 is the mole fraction of the entering gas.
- y_2 is the mole fraction of the exiting gas.
- x_1 is the mole fraction of the exiting liquid.
- x_2 is the mole fraction of the entering liquid.

The height of each transfer unit is given by:

$$HTU = \frac{G_m}{\rho_G K_G a_w}$$

- G_m is the superficial mass velocity of gas.
- ρ_G is the gas phase density.
- K_G is the overall mass transfer coefficient for the gas phase.
- a_w is the area of packing wetted by the flowing liquid per unit volume of packed bed.

The wetted area a_w is calculated from a correlation developed by Onda et al. (1968):

$$\frac{a_w}{a_t} = 1 - \exp \left[-1.45 \left(\frac{\sigma_c}{\sigma_L} \right)^{0.75} (Re_L)^{0.1} (Fr_L)^{-0.05} (We_L)^{0.2} \right].$$

- σ_c is the critical surface tension of packing material for water.
- σ_L is the water surface tension .
- Re_L is the dimensionless Reynolds number,

$$Re_L = \frac{L_m}{a_t \mu_L}.$$

- Fr_L is the dimensionless Froud number,

$$Fr_L = \frac{L_m^2 a_t}{r_L^2 g}.$$

- We_L is the dimensionless Weber number,

$$We_L = \frac{L_m^2}{r_L s_L a_t}.$$

- a_t is the total packing surface area per packed bed volume.
- L_m is the superficial mass velocity of liquid.
- μ_L is the liquid phase viscosity.
- ρ_L is the liquid phase density.

The overall mass transfer coefficient for the gas phase K_G is given by

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{m}{k_L}.$$

where,

- k_L is the mass transfer coefficient for the liquid phase.
- k_G is the mass transfer coefficient for the gas phase.

k_L and k_G are calculated from the following correlations developed by Onda et al.:

$$k_L \left(\frac{\rho_L}{\mu_L g} \right)^{0.333} = 0.0051 \left(\frac{L_m}{\mu_L a_w} \right)^{0.666} \left(\frac{\mu_L}{\rho_L D_L} \right)^{-0.5} (a_t t_p)^{0.4}.$$

$$\frac{k_G}{a_t D_G} = 5.23 \left(\frac{G_m}{\mu_G a_t} \right)^{0.7} \left(\frac{\mu_G}{\rho_G D_G} \right)^{-0.333} (a_t d_p)^{-2}.$$

- d_p is the nominal packing diameter.
- D_L is the liquid phase diffusivity.
- D_G is the gas phase diffusivity.

The Onda correlations have been verified over:

$0.5 < L_m < 0.43 \text{ kg / m}^2 \text{ sec}$, $0.017 < G_m < 1.7 \text{ kg / m}^2 \text{ sec}$,

with packing materials ranging in nominal diameter from 10 to 55 mm.

The diameter of the packed bed as well as the pressure drop are calculated using the flooding and pressure drop correlation, shown in Figure 6.34 of Treybal (1980).

In Rating Mode, the user specifies the dimensions of the column and the system calculates the pressure drop and optionally the removal efficiency of the various components.

References

1. McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill.
2. Treybal, R.E. (1980). *Mass-Transfer Operations*, McGraw-Hill.
3. Onda K., H. Takeuchi H., and Y. Okumoto. (1968). *J. Chem. Eng. Japan*, 1, 1, p. 56-62.

Stripping Operation

In stripping, a volatile solute is removed from a liquid mixture by bringing the liquid into contact with an inert gas. It is the reverse operation of gas absorption.

Material Balances

In Design Mode, the material balances are specified by the user (as % Removed) and the separation specifications drive the equipment sizing calculation (see Equipment sizing). In Rating Mode, the removal efficiency (% removed) is either set by the user or calculated by the model.

Equipment Sizing

In Design Mode, the height Z of the column is calculated from the height of the transfer unit HTU and the number of transfer units NOG :

$$Z = HTU * NOG$$

The number of transfer units is given by:

$$N_{OL} = \frac{S}{S-1} \ln \left[\frac{\frac{x_2 - y_1/m}{x_1 - y_1/m} (S-1) + 1}{S} \right]$$

- S is the stripping factor defined as

$$S = \frac{mG}{L}$$

- L is the volumetric flow rate of the liquid stream.
- G is the volumetric flow rate of the gas stream.
- m is the slope of the equilibrium curve (equal to the Henry's law constant for dilute solutions).
- y_1 is the mole fraction of the entering gas.
- y_2 is the mole fraction of the exiting gas.
- x_1 is the mole fraction of the exiting liquid.
- x_2 is the mole fraction of the entering liquid.

The height of each transfer unit is given by:

$$HTU = \frac{L_m}{r_L K_L a_w}$$

- L_m is the superficial mass velocity of liquid.
- r_L is the liquid phase density.
- K_L is the overall mass transfer coefficient for the liquid phase.
- a_w is the area of packing wetted by the flowing liquid per unit volume of packed bed.

The wetted area a_w is calculated from a correlation developed by Onda et al. (1968), presented in the absorber model. The overall mass transfer coefficient for the liquid phase K_L is given by:

$$\frac{1}{K_L} = \frac{1}{m k_G} + \frac{1}{k_L}.$$

- k_L is the mass transfer coefficient for the liquid phase.
- k_G is the mass transfer coefficient for the gas phase.
- k_L and k_G are calculated from correlations developed by Onda et al. (See absorber model).

The diameter of the packed bed as well as the pressure drop are calculated using the flooding and pressure drop correlation, shown in Figure 6.34 of Treybal (1980).

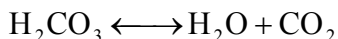
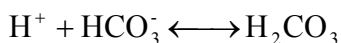
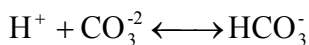
In Rating Mode, the user specifies the dimensions of the column and the system calculates the pressure drop and optionally the removal efficiency of the various components.

References

1. McCabe W. L., J. C. Smith, and P. Harriott. (1993). *Unit Operations of Chemical Engineering*, McGraw-Hill.
2. Treybal, R.E. (1980). *Mass-Transfer Operations*, McGraw-Hill.
3. Onda K., H. Takeushi H., and Y. Okumoto. (1968). *J. Chem. Eng. Japan*, 1, 1, p. 56-62.

Degasification

In water purification, degasifiers are used to remove CO₂ that is present in acidic waters that leave the cation exchange beds (Meltzer, 1993). More specifically, the use of hydrogen-cation exchange resin substitutes hydrogen ions for the calcium and magnesium ions removed from the solution. The enrichment of the treated water with hydrogen ions (its acidification) converts the bicarbonate and carbonate ions to carbonic acid. The acid decomposes readily to release carbon dioxide.



Degasifiers are packed towers, similar to strippers and absorbers. The removal of the generated CO₂ is accomplished by blowing air (or some other gas into the column) or by applying vacuum. The latter approach is followed in the semiconductor and pharmaceutical industries where general and microbiological contamination of the water (by the stripping gas) is a concern. Vacuum degasifiers substitute vacuum for the sweeping air stream to remove carbon dioxide from the thin films of water permeating the packing of the deaeration towers. This removes the threat of microbiological contamination but substitutes other disadvantages, among them the high capital and energy costs of vacuum pumps, the need for ASME-code vessels to withstand the vacuum, and requirements for the stainless steel construction and piping necessary to avoid contamination by iron, etc.

Material and Energy Balances

This is a very simple model. The material balances are based on the removal percentage of the gaseous components that is specified by the user. To account for utilities (steam for vacuum generation, electricity for pumps, and cooling water for vacuum pumps) the user can specify specific (based on flowrate or amount of water treated) or absolute values.

Equipment Sizing

In Design Mode of calculation, the program divides the volumetric throughput by the rated flux of the equipment to estimate its cross sectional area and diameter. If the calculated diameter exceeds its maximum possible value (part of the equipment description), multiple units are assumed that operate in parallel. The "Height to Diameter" ratio is used to estimate the column height.

Equipment Capacity Utilization

Dividing the operating flux by the rated flux yields the equipment capacity utilization.

References

Meltzer, T.H. (1993). "High Purity Water Preparation for the Semiconductor, Pharmaceutical, and Power Industries", Tall Oaks Publishing, Littleton, Colorado.

Storage Operations

Batch Storage

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Batch Storage In Plastic Bag

This operation handles storage of material in disposable bags and other plastic containers. Storage in plastic bags is quite common in bio-processing when small amounts of material harvested over a period of time are processed at a later point. Typically, the harvested material is frozen in the bag and kept refrigerated until the time comes to be processed. At that point, the material is thawed and the contents of several bags are combined to create a lot for downstream processing). The user can specify the cost of the plastic bag/container and its replacement frequency in terms of time or cycles. The system will calculate the annual amount of bags/containers needed and their cost.

Equipment Sizing

In terms of sizing, each plastic bag/container is treated as a vessel. In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated bag/container volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total bag/container volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to bag/container volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Continuous Storage

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

where (F) is the feed volumetric flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Batch Solids Storage

This unit operation is used to model batch-wise storage of bulk solids in a silo.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The specified or retrieved bulk density of the stored material is used to calculate the bulk volume of the stored material from its mass. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Equipment Purchase Cost

Equipment purchase cost is based on total vessel volume and material of construction.

Continuous Solids Storage

This unit operation is used to model storage of a continuous flow of bulk solids in a silo.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. The specified or retrieved bulk density of the stored material is used to calculate the volumetric flowrate of the stored material from its mass flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Equipment Purchase Cost

Equipment purchase cost is based on total vessel volume and material of construction.

Junction Box Mixing

Junction boxes combine wastewater streams prior to entering a treatment plant.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. Dividing the vessel volume by the tank depth yields the tank surface area. If the calculated surface area exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total surface area equal to the calculated.

In Rating Mode, the user specifies the vessel area and depth, the number of units, and the working to vessel volume ratio and the program calculates the residence time.

VOC Emission Calculations

Junction boxes are usually open to the atmosphere and VOC emissions occur in the same manner as emissions from quiescent surface tanks (see Clarification Model for a detailed description of the emission calculations from quiescent tanks), except that the liquid phase mass transfer coefficient is given by the following empirical equation (EPA, 1994):

$$k_{\lambda} = 1.41 \times 10^{-14} \left(\frac{v^{0.67}}{d^{0.85}} \right) \left(\frac{D_w}{D_{\text{ether}}} \right)^{0.83}$$

where v is the wastewater velocity in (cm/s) and is calculated by dividing the wastewater flowrate by both the depth of the liquid inlet flow into the junction box, d , and width of the junction box (or, the square root of the area of the liquid surface). D_w and D_{ether} are the diffusivities of the VOC and ether (reference component) in water respectively. The depth, d , can be estimated in two different ways depending on the location of the inlet pipe. If the pipe is submerged below the surface of the wastewater, the depth is equal to the pipe's internal diameter plus the distance the pipe is submerged under the surface of the liquid in the junction box. If the location of the wastewater discharge is at the surface of the liquid in the junction box, then the depth of flow is considered to be half of the pipe's internal diameter. The calculation of the gas phase mass transfer coefficient, k_g , as well as the rest of the VOC emission calculations are identical to those of the clarifier.

References

U. S. Environmental Protection Agency (EPA). 1994. "Air Emissions Models for Waste and Wastewater," *Rep. EPA-453/R-94-080A*. Research Triangle Park, NC: Office of Air Quality Planning and Standards.

Equalization

Flow equalization is the damping of flowrate variations so that a constant or nearly constant flowrate is achieved. Equalization tanks during wastewater treatment can be placed either "in-line" (major flow damping) or "off-line" (minor flow damping). The principal benefits of flows equalization are: (a) biological treatment is enhanced because shock loadings are eliminated or minimized, inhibiting substances are diluted and pH is stabilized; (b) the effluent quality and thickening performance of secondary sedimentation tanks following biological treatment is improved through constant solids loading; (c) effluent-filtration surface-area requirements are reduced, filter performance is improved and more uniform filter-backwash cycles are possible; and (d) in chemical treatment, damping of mass loading improves chemical feed control and process reliability.

The volume requirements are found by determining the biggest difference between the highest volume accumulation in the tank and the lowest volume accumulation in the tank, as calculated from the supplied experimental measurements of inflow in several time intervals (ideally around a full day, or 24h period). In practice the actual tank volume will be larger than the theoretically determined to account for the following factors: (a) Continuous operation of aeration and mixing equipment will not allow complete drawdown, although special structures can be built, (b) Volume must be provided to accommodate the concentrated plant recycle streams that are expected, if such flows are returned to the equalization basin, and (c) Some contingency should be provided for unforeseen changes in the incoming flow.

Equipment Sizing

In Design Mode of calculation the model predicts the minimum required liquid volume for equalization based on the sampled data supplied (in the constant outlet flow mode) or based on the total liquid volume supplied (in the mode where outlet flow is equal to input flow). Then based on the liquid to total volume ratio, it estimates the tank volume, surface area and number of units.

In summary, an equalization tank set in design mode calculates as follows:

Given

- Sample Measurements of Inlet Flow and Concentration
- Operation Mode (constant outlet flow, or constant storage volume)
- Tank Shape (rectangular vs. circular)
- Tank Depth
- Liquid to Total Ratio and,
- Maximum Surface Area

Calculate

- Number of Units Required
- Surface Area for Each Unit

In Rating Mode of calculation, the system considers the supplied value for surface area, number of units and depth (or in the case of constant storage flow, total liquid storage) and based on the supplied measurements decides if there's enough equalization volume (in case outlet flow is considered to be equal to the time average of the inlet flow measurements). Note that in case where the operating mode is set to "outlet flow = inlet flow" (constant storage volume) the equalization criterion is always satisfied; also, in that case the user cannot set the surface area (otherwise the system becomes over-specified).

In summary, an equalization tank set in rating mode calculates as follows:

Given

- Sample Measurements of Inlet Flow and Concentration
- Operation Mode (constant outlet flow, or constant storage volume)
- Tank Shape (rectangular vs. circular)
- Tank Depth
- Liquid to Total Ratio and,
- Number of Units Required
- Surface Area (unless mode is set to constant storage flow)

Calculate

- Feasibility (unless mode is set to constant storage flow)

VOC Emission Calculations

For volatile organic compound (VOC) emission calculations, it is assumed that the equalizer behaves like a quiescent tank. The calculations are identical to those of the Clarification Model.

References

1. Metcalf & Eddy, Inc. 3rd Ed.(1991) *Wastewater Engineering*, McGraw-Hill, Inc.
2. D. W. Sundstrom, H. E. Klei, (1980) *Wastewater Treatment*, Prentice Hall, Inc..

Solids Storage in a Hopper

This unit operation is used to model storage of a continuous flow of bulk solids in a hopper.

Equipment Sizing

In Design Mode of calculation, the user specifies the residence time (t_R) and the working to vessel volume ratio. The working (liquid) volume (V_w) and the vessel volume (V) are calculated using the following equations:

$$V_w = F * t_R$$

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

Where (F) is the feed volumetric flowrate. The specified or retrieved bulk density of the stored material is used to calculate the volumetric flowrate of the stored material from its mass flowrate. If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple, identical units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume, the number of units, and either the residence time or the working to vessel volume ratio. When the residence time is specified, the system calculates the working to vessel volume ratio using the above equations and checks to make sure that the calculated value is between the minimum and maximum working to vessel volume ratio. When the working to vessel volume ratio is specified, the system calculates the residence time using the above equations.

If this unit operates in a batch plant, the feed flowrate F is calculated by dividing the volume of material that needs to be processed per cycle by the process time.

Heating & Cooling Operations

Heat (in a Heater)

This operation models the increase in temperature of a continuous flow or batch stream. The heat is provided by an appropriate heating agent that is specified by the user.

Energy Balance and Equipment Sizing

The energy balance is represented by the following two equations:

$$Q = U A \Delta T = m C_p \Delta T,$$

where,

- Q is the heating duty, kcal / hr.
- U is the overall heat transfer coefficient, kcal / hr -°C - m² .
- ΔT is the mean temperature difference driving force, °C.
- A is the heat transfer area, m².
- m is the stream mass flow, kg/hr.
- C_p is the specific heat capacity of the stream, kcal/kg-°C.

U is always specified by the user and m and C_p are always calculated based on the stream flow and composition. When the user specifies the exit temperature (equivalent to specifying the value of ΔT), the above equations are solved for Q and A. When the user specifies the value of Q, the above equations are solved for ΔT and A. If the calculated A exceeds the maximum heat transfer area, the system assumes multiple units operating in parallel with a total heat transfer area equal to the calculated.

In Rating Mode, the calculated heat transfer is compared with the specified and if it is smaller, the user is advised to increase the heat transfer area and/or the number of units.

Heat (in an Electric Heater)

This operation models the increase in temperature of a continuous flow or batch stream. The heat is provided by electricity.

Energy Balance and Equipment Sizing

The energy balance is represented by the following equation:

$$P = \eta \, m \, C_p \, \Delta T,$$

where,

- P is the electric power, kW.
- η is the heat transfer efficiency.
- ΔT is the temperature change, °C.
- m is the stream mass flow, kg/hr.
- C_p is the specific heat capacity of the stream, kcal/kg-°C.

In Design Mode, the user specifies the desired exit temperature (which is equivalent to specifying the value of ΔT) and the above equation is used to calculate the required electric power, P . If the calculated value of P exceeds the Max Power, the system assumes multiple units operating in parallel. In Rating Mode, the user specifies the value of P and the above equation is solved for ΔT to calculate the exit temperature.

Cool (in a Cooler)

This operation models the decrease in temperature of a continuous flow or batch stream. The heat is removed by an appropriate cooling agent that is specified by the user.

Energy Balance and Equipment Sizing

The energy balance is represented by the following two equations:

$$Q = U A \Delta T = m C_p \Delta T,$$

where,

- Q is the cooling duty, kcal / hr.
- U is the overall heat transfer coefficient, kcal / hr -°C - m² .
- ΔT is the mean temperature difference driving force, °C.
- A is the heat transfer area, m².
- m is the stream mass flow, kg/hr.
- C_p is the specific heat capacity of the stream, kcal/kg-°C.

U is always specified by the user and m and C_p are always calculated based on the stream flow and composition. When the user specifies the exit temperature (equivalent to specifying the value of ΔT), the above equations are solved for Q and A. When the user specifies the value of Q, the above equations are solved for ΔT and A. If the calculated A exceeds the maximum heat transfer area, the system assumes multiple units operating in parallel with a total heat transfer area equal to the calculated.

In Rating Mode, the calculated heat transfer is compared with the specified and if it is smaller, the user is advised to increase the heat transfer area and/or the number of units.

Cool (in an Electric Cooler)

This operation models the decrease in temperature of a continuous flow or batch stream. The cooling is achieved using electricity.

Energy Balance and Equipment Sizing

The energy balance is represented by the following equation:

$$P = m C_p \Delta T / \eta$$

where,

- ⇒ P is the electric power, kW.
- ⇒ η is the power efficiency.
- ⇒ ΔT is the temperature change, °C.
- ⇒ m is the stream mass flow, kg/hr.
- ⇒ C_p is the specific heat capacity of the stream, kcal/kg-°C.

In Design Mode, the user specifies the desired exit temperature (which is equivalent to specifying the value of ΔT) and the above equation is used to calculate the required electric power, P. If the calculated value of P exceeds the Max Power, the system assumes multiple units operating in parallel. In Rating Mode, the user specifies the value of P and the above equation is solved for ΔT to calculate the exit temperature.

Cool (in a Cooling Tower)

A cooling tower is used as a specialized heat exchanger; the two fluids involved are water and air. During this operation water is sprayed into the tower from the top and air enters through the side-wall (crossflow configuration). A percentage of the water is vaporized which results in heat transfer from the liquid to the gas stream. The modeling of the cooling in tower operation is very specific to this process, and calculations will not be performed or be accurate for large deviations from the typical cooling tower operation conditions.

The inlet water stream, may contain some contaminants. If these are volatile, emission calculations can be performed. If the composition of water stream is specified so that water is less than 95 %, calculations will not be accurate, even though they are still performed. If the inlet gas stream contains other components in concentrations > 5 % calculations will not be accurate, even though they are still performed.

A classical treatment of cooling tower design (with the basic assumptions), as described in references 1-3 is followed in the model:

The Cooling Tower Range is calculated from:

$$\text{Range} = T_{wl} - T_{wo},$$

where T_{wl} and T_{wo} are the input (hot) and output (cold) water temperatures. The Approach Temperature is calculated from:

$$\text{Tap} = T_{wo} - T_{wb},$$

where T_{wb} is the Air wet bulb temperature.

The flowrate of the input water (L) is flowrate of the water input stream and the flowrate of the input air (G) is calculated from the water to air ratio (L/G) which is either set by user (design mode) or calculated by the model (rating mode). The required flow of the air stream, is propagated backwards, through the network of connectivity.

The maximum water to air ratio, for feasible cooling tower operation (L/G_{\max}) is calculated based on the above variables, following a graphical method as described in references (1-3). In design mode the user specifies L/G, and if this is greater than L/G_{\max} a warning message will come up prompting for reducing its value.

Energy Balance:

The energy balance is represented by the following 2 equations:

$$Q = G (H_{ao} - H_{al}) = L (T_{wo} - T_{wl}) C_{p\text{water}},$$

where Q is the cooling duty and H_{ao} , H_{al} are the enthalpy of the output and input air respectively. The cooling duty is calculated based on the second energy equation. Note that the psychotropic equations (ref. 5) are used to relate the enthalpy of air to its humidity and temperature or the wet bulb temperature (T_{wb}). In design mode the enthalpy of output air (H_{ao}) is obtained from the energy balance and the theoretical number of stages (n), or tower characteristic integral, is then calculated by the Merkel equation (ref. 1-3):

$$n = \frac{L}{G} C_{p\text{water}} \int_{H_{al}}^{H_{ao}} \frac{dT_w}{H_{a\text{Sat}} - H_a}$$

where T_w is the temperature of water (obtained from energy balance for given the air enthalpy) and $H_{a\text{Sat}}$ is the Saturation Enthalpy of air at that temperature (the temperature of the water-air interface). Since this integral applies to a counter-current configuration, a correction factor for a crossflow configuration is used (ref. 4). This theoretical number of stages is used for sizing calculations.

In rating mode the L/G is first calculated solving simultaneously the Merkel equation and the sizing correlations. The enthalpy of the output air (H_{aO}) is then calculated from the energy balance. In rating mode the Water Loading is calculated based on the input water flow rate and the area of the tower.

The temperature of output air (T_{aO}) is calculated from numerical integration the following equation:

$$\frac{dH_a}{dT_a} = \frac{(T_{Sat} - T_a)}{(H_{aSat} - H_a)}$$

where H_a and T_a represent the enthalpy and temperature of air, and T_{Sat} and H_{aSat} represent the “interface” temperature and air enthalpy, that is the water temperature and air saturation enthalpy. In order to obtain T_{Sat} and H_{aSat} for every given air temperature the energy balance and the psychotropic equations are used. The equation above is derived from a combination of the heat and a mass transfer balances and the Lewis relations therefore it is only valid for water-air systems (ref. 1-2).

Knowing the temperature and enthalpy of the input and output air, the psychotropic equations are used to calculate the humidity of the input and output air (Y_{wi} and Y_{wo}). The water uptake of the air stream represents the water evaporation rate.

Equipment Sizing

In design mode the packing height is calculated based on the Tower Characteristic Integral or (theoretical number of stages), using correlations for wood-splash bar packed towers (ref. 4). The tower area is calculated based on the water flow rate and water loading specified by the user.

References

1. Wankat, P.C. (1988). Equilibrium Staged Separations, Elsevier.
2. W.L. McCabe, Smith, J.C, and Harriot, P. (1993). Unit Operations of Chemical Engineering, McGraw-Hill.
3. R.H. Perry and Green, D.W. (1999). Perry's Chemical Engineers' Handbook, McGraw-Hill.
4. A.K.M. Mohiuddin and Kant K. (1996). *Int J. Refrig.*, 19(1), pp43-60.
5. Psychometrics, ASHRAE Handbook of Fundamentals, ASHRAE, Atlanta, GA.

Heat Exchanging

This operation models the transfer of heat from a hot to a cold stream through the use of a heat exchanger. The heat exchanger can be of Plate & Frame, Spiral, or Shell and Tube type. Several options are available for specifying performance specifications and operating conditions.

Energy Balance and Equipment Sizing

The energy balance is represented by the following equations:

$$Q = \eta U A \Delta T_{LN} = m_1 C_{p1} \Delta T_1 = m_2 C_{p2} \Delta T_2$$

where,

- Q is the heat transfer (exchange) rate, kcal / hr.
- U is the overall heat transfer coefficient, kcal / hr -°C - m² .
- ΔT_{LM} is the log mean temperature difference driving force, °C.
- η correction factor that accounts for deviations from countercurrent or co-current flow
- A is the heat transfer area, m².
- m_i is the mass flow of stream i, kg/hr.
- C_{pi} is the specific heat capacity of the stream i, kcal/kg-°C.
- ΔT_i is the temperature change of stream i, °C.

The value of U is always specified by the user. The values of m and C_p are always calculated based on the stream flows and compositions. The values of ΔT_i are calculated based on the performance specifications.

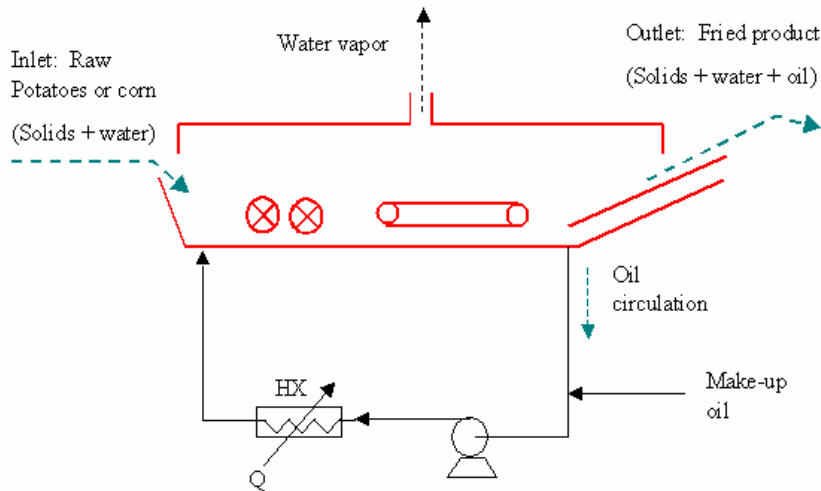
In Design Mode, the above equations are solved for A. If the calculated A exceeds the maximum heat transfer area, the system assumes multiple units operating in parallel with a total heat transfer area equal to the calculated.

In Rating Mode, the required (calculated) heat transfer area is compared with the specified and if it is smaller, the performance specifications are adjusted to feasible values.

The pressure drop variables have no impact on the sizing calculations. Simply, they are used to set the pressure of the output streams.

Frying

The purpose of this model is to simulate the industrial frying of food products, for example potato or corn chips. A schematic of continuous frying operation is shown below.



In order to fry the chips a certain amount of oil circulates through a heat exchanger, and make up oil is added to recover the oil that is lost in the product. The potato chips (or any other food product) will be modeled in SPD components in terms of their solids, water, and oil content. The user specifies the water and the oil component in the material balance tab and everything else in the product stream is considered to belong to “solids”. The fried product contains significantly lower amount of water than the raw product as part of the water contained in the food evaporates.

Material Balance:

There are 2 options available for the material balance. The user can either set the oil and water content of the product, or let that be calculated through a built in model. If the user chooses the built in model the moisture loss is calculated by the following equation:

$$Water_{In} - Water_{Out} = At + Bt^2 + Ct^3 + Dt^4 + Et^5$$

where $Water_{In}$ is the water mass fraction in the input product stream and $Water_{Out}$ is the water fraction in the output product stream, t is the residence time in the fryer (specified by the user) and A, B, C, D, E are user specified model parameters. The oil-uptake by the product is calculated by:

$$Oil_{Out} = F \left(1 - \frac{Water_{Out}}{Water_{In}} \right)$$

where Oil_{out} is the mass fraction of the oil component in the output product stream (fried product) and F is a user-specified factor.

Energy Balance:

There are two options for the energy balance. The user can either set the outlet temperature (of product and recirculating oil) and let the heat transfer efficiency be calculated by the program, or set the heat transfer efficiency and let this outlet temperature be calculated. The recirculation rate, and the inlet oil temperature (that is the temperature of the oil after it goes through the heat exchanger) needs to be specified by the user.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Heat Sterilization

The purpose of this model is to simulate death kinetics in the holding tube of a continuous sterilizer.

Death Kinetics

The death of microorganisms and spores in the holding tube of a continuous heat sterilizer is represented by the following equation (Wang et al, 1979):

$$-\frac{dN}{dt} = k N ,$$

where N is the concentration of viable organisms in number/liter, k is the specific death rate constant in sec^{-1} , and t is time in minutes. At $t = t_0$, $N = N_0$. The specific death rate (k) is related to sterilization temperature by an Arrhenius type of equation:

$$k = A \exp\left(-\frac{\Delta E}{R T}\right),$$

where A is the frequency factor in sec^{-1} , ΔE is the activation energy of death in cal/mole, R is the gas constant in cal/mole-K, and T is the absolute temperature in K. The program provides good default values for A , ΔE , R , and T , which the user has the option to modify.

Since actual plug flow through the holding tube of a continuous sterilizer is never achieved, an axial dispersion model is assumed to account for residence time distribution. Solving the material balance equation, we get:

$$\frac{N}{N_0} = \frac{4\delta \exp\left(\frac{N_{pe}}{2}\right)}{(1 + \delta^2) \exp\left(\frac{N_{pe}\delta}{2}\right) - (1 - \delta)^2 \exp\left(\frac{N_{pe}\delta}{2}\right)},$$

$$\text{where } \delta = \sqrt{1 + \frac{4N_R}{N_{pe}}}, N_R = \frac{kL}{U}, N_{pe} = \frac{UL}{D_z}.$$

U is the average medium velocity (m/sec), L is the length of the holding tube (m), D_z is the axial dispersion coefficient (m^2/sec). D_z is estimated as a function of the Reynolds number from the following equation:

$$\frac{D_z}{\mu/\rho} = 6.0936 * 10^5 - 1.2324 * 10^5 \ln(\text{Re}) + 6279.2 [\ln(\text{Re})]^2,$$

where μ is the liquid viscosity (kg/m-s) and ρ is the liquid density (kg/m^3). This equation was derived by curve fitting experimental data (Figure 40, Levenspiel, 1972). The user also has the option to select a simplified plug-flow model.

Equipment Sizing

In design mode of calculation, the tube diameter (d_t) and the sterility level (N/N_0) are specified and the equations are solved iteratively to estimate the required tube length (L). In rating mode

of calculation, the tube diameter (d_t) and length (L) are specified and the equations are solved to estimate the sterility level (N/N_0)

The size estimation of the heat exchangers that are used for energy conservation as well as the estimation of heating and cooling duties are based on intermediate and final temperatures of various streams that are specified by the user.

Capital Cost

The equipment purchase cost includes the cost of the holding tube along with its insulation, the heat exchangers for energy conservation, and the cost of the pumps. It is function of throughput.

References

1. Wang, D. I. C., C. L. Cooney, A. L. Demain, P. Dunnill, A. E. Humphrey, and M. D. Lilly (1979). Fermentation and Enzyme Technology, John Wiley & Sons.
2. Levenspiel, O. (1972). Chemical Reaction Engineering, 2nd edition, John Wiley & Sons.

Mixing Operations

Mixing (Bulk Flow)

This unit operation mixes two or more (up to 9) bulk streams and creates an outlet stream. The operating throughput of the step is calculated based on the flow of the output stream.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Custom Mixing

Oftentimes, during the design of a new process, it is required that we either dilute or concentrate a process stream by mixing it with another stream. As typically a designer will have a goal in mind for the mixing, the flowrate of the mix-in inlet has to be determined during simulation. This model will allow users to express such process design constraints directly. Note that the composition of the adjustable add-in stream must be set by the user before the simulation starts.

Under certain circumstances, the model will fail to determine a value for the adjustable mix-in stream that will meet the constraint set by the user. These circumstances are described below:

1. The output mass flowrate is set to a value that turns out to be lower than the process (bottom) stream's flowrate.
2. The output volumetric flowrate is set to a value that turns out to be lower than the process (bottom) stream's volumetric flowrate.
3. The concentration (or mass fraction) of the design component set for the output stream does not fall in between the concentration (or mass fraction) of the same component in the process (bottom) stream and the adjustable mix-in.

If any of the above conditions is detected during simulation, a warning message will appear. In order to remedy the situation, you must either relax the mixing specification or adjust some process conditions upstream that will change the flowrate and/or the concentration/mass fraction of the design component in the process input stream.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Mixture-Preparation

Oftentimes, during the design of a new process, it is required that we mix a number of streams in order to create a mixture with certain composition. This operation simulates an intelligent mixer that automatically will adjust the (bulk) flow of its input streams (up to 5) in order to meet a user-specification describing the output composition and flow. If there are n input streams to the procedure then $n-1$ key components and their concentration needs to be specified. The output mass (or volume) flow can be specified by the user, set by the downstream process (via a back-propagation request), or calculated based on the “known” flow of a fixed input stream. An overall mass balance, and $n-1$ component mass balances are solved simultaneously in order to determine the inlet stream flow rates.

Under certain circumstances, the model will fail to determine a value for the adjustable inlet streams and a warning will message will appear, explaining why the specifications set are unachievable and giving suggestions on how to remedy the situation.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

2-Stream Mixing (Discrete Flow)

To mix (combine) two or more discrete streams, the discrete entities in all of them must be identical. Two discrete entities are considered identical if all of the following attributes are the same: Name, Bulk Amount per Entity, Bulk Composition, Purchasing Price, and Selling Price.

The operating throughput (in entities/min) of the step is calculated based on the flow of the output stream.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Tumble Mixing

This unit operation is used to model batch-wise mixing of bulk solids in a tumble mixer.

Equipment Sizing

In Design Mode of calculation, the user specifies the working to vessel volume ratio (through the Volumes tab) and the system sets the working (liquid) volume (V_w) equal to the volume of material that is processed per cycle. The specified or retrieved bulk density of the stored material is used to calculate the bulk volume of the stored material from its mass. The number of cycles per batch is specified through the Scheduling tab. The vessel volume (V) is calculated using the following equation:

$$V = V_w / (\text{Working to Vessel Volume Ratio})$$

If the calculated vessel volume exceeds its maximum possible value (specified through the Equipment tab), the system assumes multiple (identical) units operating in parallel with a total vessel volume equal to the calculated.

In Rating Mode, the user specifies the vessel volume and the number of units. The system calculates the working to vessel volume ratio and warns the user if its value is outside of its minimum and maximum limits.

Splitting Operations

Splitting (Bulk Flow)

This operation splits the flowrate of a bulk stream into two streams based on user-defined split fractions.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Component Splitting

This operation model splits the component flowrates of a bulk stream into two or more (up to 9) streams based on user-defined component split fractions.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

n-Way Component Splitting

This operation splits the component flowrates of a bulk stream into two or more (up to 9) streams based on user-defined component split fractions.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Custom Splitting

Oftentimes, during the design of a new process, it is required that we separate the process stream into two others. As typically a designer will have a goal in mind for the splitting, the split fraction is not known a-priori but often depends on the actual flow conditions of the process stream itself. This model will allow users to express such process design constraints directly.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Flow Distribution

This operation sets and distributes the flowrate of a bulk input stream into one or more streams (up to 3, 5 or 10). The flowrate of each output streams is either set by the user or the downstream process through a Back Propagation Request. The flowrate of the input streams is set to be equal to the sum of the output stream flow and it is also back propagated through the network of connectivity.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

2-Way Splitting (Discrete Flow)

To split the flow of discrete entities into two streams. The operating throughput (in entities/min) of the step is calculated based on the flow of the input stream.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

n-Way Splitting (Discrete Flow)

To split the flow of discrete entities into N streams. The operating throughput (in entities/min) of the step is calculated based on the flow of the input stream.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Size Reduction Operations

Shredding (Bulk)

This unit operation model simulates shredding (size reduction) of bulk solids.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/kg-h). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Shredding (Discrete)

This unit operation model simulates shredding (size reduction) of discrete solid objects.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/kg-h). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Grinding (Bulk)

This unit operation model simulates grinding (size reduction) of bulk solids.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/kg-h). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Grinding (Discrete)

This unit operation model simulates grinding (size reduction) of discrete solid objects.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/kg-h). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Formulation & Packaging Operations

Extrusion

This unit operation simulates extrusion of polymeric resins. It also can be used to model extrusion of foods and other products.

Equipment Sizing

If the equipment size option is in Design Mode, the following equation is solved for D to calculate the screw diameter (Rosato and Rosato, p. 165):

$$R = \alpha D^2 h g N$$

Where R is the mass throughput [kg/h], D is the screw diameter [cm], h is the depth of the metering section [cm], g is the specific gravity of the resin, N is the screw rpm, and α is a constant the value of which depends on the units of the other variables. If the calculated diameter exceeds the maximum screw diameter, then, the system assumes multiple, identical units operating in parallel with a screw diameter of less than the maximum. In Rating Mode, the screw diameter (D) is specified and the above equation is solved for N to calculate the screw rotational velocity. If the calculated screw rpm exceeds the maximum allowable value, a warning message is displayed advising the user to increase the number of units operating in parallel and/or reduce the operating throughput.

Electricity Cost

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/kg-h). In the second case, the specific power requirement times the mass operating throughput yields the power consumption.

References

Donald V. Rosato and Dominick V. Rosato, "Injection Molding Handbook", 2nd Edition, Chapman Hall.

Blow Molding

This unit operation simulates molding of polymeric resins for the formation of bottles and other plastic objects. The primary objective of this model is to calculate the output capacity of the step based on the dimensions and thickness of the part, the physical properties of the resin, and the molding operating conditions. A secondary objective is to estimate the cost of the mold and the operating expenses associated with this step.

Part Mass / Volume and Shot Weight

The user specifies either the mass or the volume of the molten resin that makes up the molded object. The conversion from mass to volume and vice-versa is done using the density of the resin. The specified part mass or volume must account for any extra material removed during trimming and/or reaming. Please note that in this version of Pro-Designer, the density and the thermal diffusivity of the resin are properties local to the molding process steps. In future versions of the program, the values of these properties will be retrieved from the application component databank.

The shot weight (weight of material fed into the molding unit per cycle) is equal to the number of cavities times the part weight.

Output Capacity

The output capacity of the unit is either specified by the user (based on vendor quotations) or calculated based on the part cycle time using the following equations:

$$(\text{Output Capacity}) = (\text{Number of Cavities per Mold Set}) / (\text{Part Cycle Time})$$

Where

$$(\text{Part Cycle Time}) = (\text{Part Cooling Time}) + (\text{Blow Time}) + (\text{Mold Open-Close-Eject Time})$$

The values of Blow Time and Mold Open-Close-Eject Time are machine-dependent and are always specified by the user. The Part Cooling Time is either specified by the user or calculated by the system using the following equation (Rosato and Rosato, p. 299):

$$(\text{Part_Cooling_Time}) = \frac{-(2t)^2}{2\pi\alpha} \ln \left[\frac{\pi (T_r - T_m)}{4 (T_c - T_m)} \right]$$

Where t is the maximum critical wall thickness, α is the thermal diffusivity of the resin, T_r is the ejection temperature, T_m is the mold temperature, and T_c is the melt temperature.

The Operating Output is calculated by dividing the feed flowrate by the amount of mass per part. The ratio of Operating Output over Output Capacity yields the Capacity Utilization. If the Capacity Utilization is over 100%, the user is advised by the system to either reduce the feed flowrate or increase the number of identical units that operate in parallel. Please note that a single molding icon can represent multiple molders (of the same capacity) operating in parallel. To represent that, you simply type an appropriate value for the Number of Units in the Equipment Tab.

Mold Dimensions

The dimensions of each mold cavity are estimated based on the mold to part dimension ratios that the user specifies (e.g., Mold Width / Part Width = 1.5). The total mold volume is set equal to the volume of a cavity times the number of cavities.

Mold Cost

The total cost per mold set is equal to the sum of the engineering design cost and the material and machining cost. The material and machining cost, in turn, accounts for the cost of

machining, the cost of neck rings, and the cost of the metal material. The machining cost is either specified by the user or calculated by the system based on the machining difficulty (which is specified by the user) and other mold attributes. The material cost is estimated based on the total mold weight and the unit cost of material (\$/kg). Molds are usually made of stainless steel or aluminum alloys.

The cost of the mold can contribute to cost of consumables if the "Consider cost associated with mold replacement" box is checked. Molds are usually replaced every 2-5 year of operation (specified by the replacement frequency variables). The annual consumable cost of a mold is estimated by dividing its total cost by its operating lifetime.

A mold also can contribute to capital investment if the "Capitalize Cost of First Mold Set" box is checked. In that case, the mold cost is added to the equipment (molder) cost and it contributes to capital investment and other cost that depend on capital investment (e.g., maintenance, insurance, local taxes, etc.).

Electricity Cost

To account for electricity consumption, the user can specify the power requirement (in kW). Please note that this power requirement pertains to the molding operation only and it does not include the power requirement for the extruder. The extruder power demand is specified as part of the extrusion step.

References

Donald V. Rosato and Dominick V. Rosato, "Injection Molding Handbook", 2nd Edition, Chapman Hall

Injection Molding

This unit operation simulates injection molding of polymeric resins for the formation of plastic objects. The primary objective of this model is to calculate the output capacity of the step based on the dimensions and thickness of the part, the physical properties of the resin, and the molding operating conditions. A secondary objective is to estimate the cost of the mold and the operating expenses associated with this step.

Part Mass / Volume and Shot Weight

By default, the system calculates the part mass and volume based on the dimensions of the molded object. However, the user also has the option to specify either the mass or the volume of the molten resin that makes up the molded object. The conversion from mass to volume and vice-versa is done using the density of the resin. The specified part mass or volume must account for any extra material removed during trimming and/or reaming. Please note that in this version of Pro-Designer, the density and the thermal diffusivity of the resin are properties local to the molding process steps. In future versions of the program, the values of these properties will be retrieved from the application component databank.

The shot weight (weight of material fed into the molding unit per cycle) is equal to the number of cavities times the part weight.

Output Capacity

The output capacity of the unit is either specified by the user (based on vendor quotations) or calculated based on the part cycle time using the following equations:

$$(\text{Output Capacity}) = (\text{Number of Cavities per Mold Set}) / (\text{Part Cycle Time})$$

Where

$$(\text{Part Cycle Time}) =$$

$$= (\text{Part Cooling Time}) + (\text{Injection Time}) + (\text{Hold Time}) + (\text{Clamp Open-Close-Eject Time})$$

The values of Injection Time, Hold Time and Clamp Open-Close-Eject Time are machine-dependent and are always specified by the user. The Part Cooling Time is either specified by the user or calculated by the system using the following equation (Rosato and Rosato, p. 299):

$$(\text{Part_Cooling_Time}) = \frac{-(t)^2}{2\pi\alpha} \ln \left[\frac{\pi (T_r - T_m)}{4 (T_c - T_m)} \right]$$

Where t is the maximum critical wall thickness, α is the thermal diffusivity of the resin, T_r is the heat distortion temperature, T_m is the mold temperature, and T_c is the melt temperature.

The Operating Output is calculated by dividing the feed flowrate by the amount of mass per part. The ratio of Operating Output over Output Capacity yields the Capacity Utilization. If the Capacity Utilization is over 100%, the user is advised by the system to either reduce the feed flowrate or increase the number of identical units that operate in parallel. Please note that a single molding icon can represent multiple molders (of the same capacity) operating in parallel. To represent that, you simply type an appropriate value for the Number of Units in the Equipment Tab.

Mold Dimensions

The number of cavities Top to Bottom times Left to Right times the number of stacks per mold set (1 for single face, 2 for stack of two, or 4 for stack of four) yields the total number of cavities per mold set. The mold dimensions are calculated as a function of part height, number of

cavities (top to bottom and left to right), horizontal movement, and type of mold (e.g., single face, stack of two, or stack of four).

Mold Cost

The total cost per mold set is equal to the sum of the engineering design cost, the material and machining cost, and the hot runner cost. The material and machining cost, in turn, accounts for the cost of machining and the cost of the metal material. The machining cost is either specified by the user or calculated by the system based on the machining difficulty (which is specified by the user) and other mold attributes. The material cost is estimated based on the total mold weight and the unit cost of material (\$/kg). Molds are usually made of stainless steel or aluminum alloys. The hot runner cost is estimated as a function of the number of cavities and the type of runner.

The cost of the mold can contribute to cost of consumables if the "Consider cost associated with mold replacement" box is checked. Molds are usually replaced every 2-5 year of operation (specified by the replacement frequency variables). The annual consumable cost of a mold is estimated by dividing its total cost by its operating lifetime.

A mold also can contribute to capital investment if the "Capitalize Cost of First Mold Set" box is checked. In that case, the mold cost is added to the equipment (molder) cost and it contributes to capital investment and other cost that depend on capital investment (e.g., maintenance, insurance, local taxes, etc.).

Electricity Cost

To account for electricity consumption, the user can specify the power requirement (in kW). Please note that this power requirement pertains to the molding operation only and it does not include the power requirement for the extruder. The extruder power demand is specified as part of the extrusion step.

References

Donald V. Rosato and Dominick V. Rosato, "Injection Molding Handbook", 2nd Edition, Chapman Hall

Trimming

This unit operation simulates the removal of extra material from a molded object. It also can be used as a generic operation that reduces the mass of a discrete entity. The user specifies the amount of bulk material removed from each part and the system calculates the flowrate of the bulk output stream and the new bulk amount (mass/unit) of the treated entity.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Filling

This unit operation simulates the filling of a container (discrete entity) with a certain amount of bulk material. Filling is a common step in product formulation and packaging operations. The flowrate of either the bulk line (top stream) or the container line (bottom stream) is adjusted by the system to synchronize the flowrates of the two input streams. The synchronization of the two feed streams is based on the value of bulk amount per container that is specified by the user.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Assembly

This unit operation simulates the formation of a new discrete entity from the combination of two other discrete entities. For instance, it can be used to represent the addition of a pumping mechanism or a cap to a bottle. Any number of type A entities can be combined with any number of type B entities to form the new entity. The flowrate of either the top stream (type A entity) or the bottom stream (type B entity) is adjusted by the system to synchronize the flowrates of the two input streams. The synchronization is based on the number of each type of entity required per new entity.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Printing

This unit operation simulates a printing process, a common step in packaging operations. A finite amount of bulk ink is used to print a label on a discrete entity. The flowrate of either the ink line (top stream) or the entity line (bottom stream) is adjusted by the system to synchronize the flowrates of the two input streams. The demand for ink is calculated based on the amount of ink required per print which is specified by the user.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Labeling

This operation simulates the attachment of a label on a discrete entity. Labeling is a common step in packaging operations. The flowrate of either the label line (top stream) or the product entity line (bottom stream) is adjusted by the system to synchronize the flowrates of the two input streams.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Boxing/Packaging

This operation simulates the packaging of discrete entities. It can be used to represent addition of discrete items in a carton, formation of a pallet, etc. The flowrate of either the item line (top stream) or the container line (bottom stream) is adjusted by the system to synchronize the flowrates of the two input streams. The synchronization is based on the number of items that are packaged per container.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed urging the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Tableting

This operation simulates the conversion of bulk solid material into tablets or any other discrete entities. In other words, this unit is not limited to modeling the formation of medicinal tablets but it also can be used to model formation of soap bars, chocolate bars, cookies, etc. The bulk feed flowrate divided by the amount of bulk material per tablet (or discrete entity in general) yields the discrete throughput.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. . If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Transport (near) Operations

Pumping

This operation models transport of fluids using a centrifugal pump, a gear pump or a diaphragm pump.

Energy Balance and Equipment Sizing

In Design Mode, the user specifies the desired pressure change (ΔP) and the model calculates the required power supply using the following equation:

$$\text{Power} = Q \Delta P / \eta$$

Where,

- Q is the volumetric flow rate
- ΔP is the desired pressure change
- η is the total efficiency (including pump and driver efficiencies).

If the calculated power exceeds the maximum, the system assumes multiple units operating in parallel with a total power requirement equal to the calculated.

In Rating Mode, the user specifies the power supply and the number of units operating in parallel and the system calculates the pressure change.

References

Ulrich, G.D. (1984). A Guide to Chemical Engineering Process Design and Economics, John Wiley & Sons.

Centrifugal (CF) Fanning

Industrial fans are designed to move large volumes of gases at low pressure differentials.

Equipment Sizing

In Design Mode, the system calculates the number of parallel units by comparing the operating throughput with the maximum throughput. The operating throughput is equal to the volumetric flowrate of the input stream (under input stream conditions). In Rating Mode, the user specifies the number of units and the rated throughput of each unit and the system calculates the operating throughput and warns the user if its value exceeds the rated throughput.

Energy Balances

The power requirement is calculated using the following equation (Shultz, 1962):

$$Power = \frac{k}{k-1} p_1 v_1 \left[\left(\frac{p_2}{p_1} \right)^{(k-1)/k} - 1 \right]$$

$$p_2 = p_1 \left(\frac{T_2}{T_1} \right)^{(k-1)/k}$$

where,

- k is the ratio of specific heat of gas at constant pressure to specific heat of gas at constant volume (average value = 1.3),
- v_1 is the specific volume of gas at intake conditions,
- T_1 is the absolute temperature of gas at intake conditions, and
- T_2 is the absolute temperature of gas at final delivery conditions.

The user always specifies the desired pressure change (which is equivalent to specifying the value of p_2) and the above equations are used to calculate the power requirement and the outlet temperature (T_2). If the calculated T_2 exceeds the maximum exit temperature, the system calculates the required cooling duty to maintain an exit temperature equal to the maximum.

References

1. Shultz, J.M. (1962). "The Polytropic Analysis of Centrifugal Compressors", J. Eng. Power, Trans. Am. Soc. Mech. Eng., pp. 69-82 (January 1962).
2. Peters, M.S. and K.D. Timmerhaus, (1991). Plant Design and Economics for Chemical Engineers, 4th edition, McGraw-Hill, pp. 523-525.

Centrifugal (CF) Compressing

This operation models transport of gaseous materials using a centrifugal compressor.

Equipment Sizing

Compressors operate in pressure ranges and with compression ratios that often require external cooling to prevent damage to sensitive seals and metal surfaces. This physical situation falls between the isentropic and isothermal extremes and is called polytropic compression. To calculate the power requirement for polytropic compression, the equations developed by Shultz (1962) are used:

$$Power = \frac{k}{k-1} p_1 v_1 \left[\left(\frac{p_2}{p_1} \right)^{(k-1)/k} - 1 \right]$$

$$p_2 = p_1 \left(\frac{T_2}{T_1} \right)^{k/(k-1)}$$

where,

- k is the ratio of specific heat of gas at constant pressure to specific heat of gas at constant volume (average value = 1.3),
- v_1 is the specific volume of gas at intake conditions,
- T_1 is the absolute temperature of gas at intake conditions, and
- T_2 is the absolute temperature of gas at final delivery conditions.

In Design Mode, the user specifies the desired pressure change (which is equivalent to specifying the value of p_2) and the above equations are used to calculate the power requirement and the outlet temperature (T_2). If the calculated power exceeds the maximum, the system assumes multiple units operating in parallel with a total power requirement equal to the calculated. If the calculated T_2 exceeds the maximum exit temperature, the system calculates the required cooling duty to maintain an exit temperature equal to the maximum.

In Rating Mode, the user specifies the power supply and the number of units operating in parallel and the system calculates the pressure change.

References

1. Shultz, J.M. (1962). "The Polytropic Analysis of Centrifugal Compressors", J. Eng. Power, Trans. Am. Soc. Mech. Eng., pp. 69-82 (January 1962).
2. Peters, M.S. and K.D. Timmerhaus, (1991). Plant Design and Economics for Chemical Engineers, 4th edition, McGraw-Hill, pp. 523-525.

Belt Conveying (Bulk)

This unit operation simulates transport of bulk solids using a belt conveyor.

Equipment Sizing

If Design Mode, the belt width is calculated by dividing the loading rate (MT/h) by the specific loading rate (MT/h-cm). If the calculated belt width exceeds the maximum, the system assumes multiple, identical units operating in parallel with a total belt width equal to the calculated. In Rating Mode, the user specifies the number of units and their belt width and the system calculates the specific loading rate. The user always specifies the belt length.

Electricity Cost

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in W/(kg-h)-m). In the second case, the specific power requirement times the loading rate times the belt width yields the power consumption.

Belt Conveying (Discrete)

This unit operation simulates transport of discrete objects using a belt conveyor.

Equipment Sizing

If Design Mode, the belt width is calculated by dividing the loading rate (MT/h) by the specific loading rate (MT/h-cm). If the calculated belt width exceeds the maximum, the system assumes multiple, identical units operating in parallel with a total belt width equal to the calculated. In Rating Mode, the user specifies the number of units and their belt width and the system calculates the specific loading rate. The user always specifies the belt length.

Electricity Cost

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in W/(kg-h)-m). In the second case, the specific power requirement times the loading rate times the belt width yields the power consumption.

Pneumatic Conveying (Bulk)

This unit operation simulates transport of bulk solids using a pneumatic conveyor.

Equipment Sizing

If Design Mode, the pipe cross sectional area (and consequently the pipe diameter) is calculated by dividing the operating throughput (MT/h) by the specific throughput (MT/h-m²). If the calculated pipe diameter exceeds the maximum, the system assumes multiple, identical units operating in parallel with a total cross sectional area equal to the calculated. In Rating Mode, the user specifies the number of units and their pipe diameter and the system calculates the specific throughput. The user always specifies the pipe length and the system always calculates the operating throughput.

Electricity Cost

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/(MT-h)-m). In the second case, the specific power requirement times the operating throughput times the pipe length yields the power consumption.

Pneumatic Conveying (Discrete)

This unit operation simulates transport of discrete objects using a pneumatic conveyor.

Equipment Sizing

If Design Mode, the pipe cross sectional area (and consequently the pipe diameter) is calculated by dividing the operating throughput (MT/h) by the specific throughput (MT/h-m²). If the calculated pipe diameter exceeds the maximum, the system assumes multiple, identical units operating in parallel with a total cross sectional area equal to the calculated. In Rating Mode, the user specifies the number of units and their pipe diameter and the system calculates the specific throughput. The user always specifies the pipe length and the system always calculates the operating throughput.

Electricity Cost

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/(MT-h)-m). In the second case, the specific power requirement times the operating throughput times the pipe length yields the power consumption.

Screw Conveying (Bulk)

This unit operation simulates transport of bulk solids using a screw conveyor.

Equipment Sizing

If Design Mode, the pipe cross sectional area (and consequently the pipe diameter) is calculated by dividing the operating throughput (m^3/h) by the specific throughput ($\text{m}^3/\text{h}\cdot\text{m}^2$). If the calculated pipe diameter exceeds the maximum, the system assumes multiple, identical units operating in parallel with a total cross sectional area equal to the calculated. In Rating Mode, the user specifies the number of units and their pipe diameter and the system calculates the specific throughput. The user always specifies the pipe length and the system always calculates the operating throughput. The bulk density of the conveyed material is used to convert the mass throughput into volumetric throughput.

Electricity Cost

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in $\text{W}/(\text{m}^3\cdot\text{h})\cdot\text{m}$). In the second case, the specific power requirement times the operating throughput times the pipe length yields the power consumption.

Screw Conveying (Discrete)

This unit operation simulates transport of discrete objects using a screw conveyor.

Equipment Sizing

If Design Mode, the pipe cross sectional area (and consequently the pipe diameter) is calculated by dividing the operating throughput (m^3/h) by the specific throughput ($\text{m}^3/\text{h}\cdot\text{m}^2$). If the calculated pipe diameter exceeds the maximum, the system assumes multiple, identical units operating in parallel with a total cross sectional area equal to the calculated. In Rating Mode, the user specifies the number of units and their pipe diameter and the system calculates the specific throughput. The user always specifies the pipe length and the system always calculates the operating throughput. The bulk density of the conveyed material is used to convert the mass throughput into volumetric throughput.

Electricity Cost

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in $\text{W}/(\text{m}^3\cdot\text{h})\cdot\text{m}$). In the second case, the specific power requirement times the operating throughput times the pipe length yields the power consumption.

Bucket Elevation (Bulk)

This unit operation simulates elevation (vertical transport) of bulk solids using a bucket elevator.

Equipment Sizing

This unit only has Rating Mode of equipment sizing. The user always specifies the bucket width and height and the vertical lift (length).

Electricity Cost

Electricity consumption is either specified by the user or calculated by the system using the built-in model that is based on throughput and vertical lift.

Bucket Elevation (Discrete)

This unit operation simulates elevation (vertical transport) of discrete objects using a bucket elevator.

Equipment Sizing

This unit only has Rating Mode of equipment sizing. The user always specifies the bucket width and height and the vertical lift (length).

Electricity Cost

Electricity consumption is either specified by the user or calculated by the system using the built-in model that is based on throughput and vertical lift.

Transport (far) Operations

Transport

The primary objective of transportation operations is to account for and estimate the shipping cost associated with the transportation of raw materials and finished products of a manufacturing facility. The cost is estimated using the following equation:

$$\begin{aligned} \text{(Annual Transportation Cost)} &= (\text{\# of Shipments per Year}) \times \\ &\{ \\ &\quad (\text{Fixed Cost}) + \\ &\quad (\text{Quantity Dependent Cost}) \times (\text{Quantity per Shipment}) + \\ &\quad (\text{Quantity and Distance Dependent Cost}) \times (\text{Quantity per Shipment}) \times (\text{Shipping Distance}) \\ &\} \end{aligned}$$

For units that transport bulk material as well as discrete entities, the above equation is applied twice. Transportation cost is one of the cost item that appears in the Itemized Cost and Economic Evaluation reports (see Chapters 7 & 8). Transportation operations are the only process steps that can contribute to transportation cost.

Lack of Equipment – No equipment and equipment-dependent cost is associated with transportation unit operations. Actually, the transportation cost is the only type of cost associated with transportation operations. You may view transportation operations as utility-type of units that offer transportation services to a manufacturing facility. In other words, they are not full-blown unit operations.

No Scheduling Data – Transportation units lack the scheduling tab on their i/o dialog, do not require scheduling data, and do not appear on the scheduling information dialog and the Gantt chart (see Chapter 6 for information on process scheduling).

Pressure Drop (using Valves) Operations

Pressure Drop Operation (Gate Valve - Liquids)

This operation models the pressure drop of liquids flowing through a gate valve.

Equipment Sizing

Given the flow rate through the valve and the pressure drop the required valve flow capacity (C_v) is calculated:

$$C_v = Q / \sqrt{\Delta P / S.G.}$$

where:

- Q is the liquid flow rate (in Gallons per Minute)
- ΔP is the pressure drop (in psi)
- S.G is the specific gravity of medium (relative to water)
- C_v is the flow capacity of the valve. 1 C_v unit corresponds to 1 GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi.

Note that most manufacturers provide valve data (C_v vs. Diameter) in the American units system. The system does all appropriate conversions to display all variables in SI, except for the flow capacity, which is displayed in the above units (" C_v ").

In Design Mode the user specifies the pressure drop and maximum diameter. A manufacturer chart, relating C_v and Diameter is used to calculate the diameter. If the diameter exceeds the maximum the system assumes multiple units operating in parallel with a total Flow Capacity (C_v) equal to the calculated.

In Rating Mode, the user specifies the diameter and number of units. The system uses the manufacturer's chart to get the flow capacity and the resulting pressure drop.

[As the C_v vs. Diameter data may vary from manufacturer to manufacturer, the user can use the calculated Flow Capacity (C_v) for obtaining the exact diameter from any manufacturer chart.]

Pressure Drop (Globe / Butterfly Valve - Liquids)

This operation models the pressure drop of liquids flowing through a control valve (globe or butterfly)

Equipment Sizing

Given the flow rate through the valve and the pressure drop the required valve flow capacity (C_v) is calculated:

$$C_v = Q / \sqrt{\Delta P / S.G.}$$

where:

- Q is the liquid flow rate (in Gallons per Minute)
- ΔP is the pressure drop (in psi)
- S.G is the specific gravity of medium (relative to water)
- C_v is the flow capacity of the valve. 1 C_v unit corresponds to 1 GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi.

Note that most manufacturers provide valve data (C_v vs. Diameter) in the American units system. The system does all appropriate conversions to display all variables in SI, except for the flow capacity, which is displayed in the above units (" C_v ").

The fully open valve flow capacity C_{vmax} is then calculated from the % opening:

$$C_{vmax} = C_v / (\% \text{ open}).$$

In Design Mode the user specifies the pressure drop and maximum diameter. A manufacturer chart, relating C_{vmax} and Diameter is used to calculate the diameter. If the diameter exceeds the maximum the system assumes multiple units operating in parallel with a total Flow Capacity (C_{vmax}) equal to the calculated.

In Rating Mode, the user specifies the diameter and number of units. The system uses the manufacturer's chart to get the flow capacity and the resulting pressure drop.

[As the C_{vmax} vs. Diameter data may vary from manufacturer to manufacturer, the user can use the calculated Flow Capacity (C_{vmax}) for obtaining the exact diameter from any manufacturer chart.]

Pressure Drop Operation (Gate Valve - Gas)

This operation models the pressure drop of gases flowing through a gate valve. The model described below is valid for small pressure drops in gas flow. The flow capacity formula, for calculating the C_v of a valve was design for liquid flow and is expressed in "GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi". However this flow capacity (in the same units) and similar formula is used for gas flow through a valve.

Equipment Sizing

Two different pressure regimes are considered for the sizing a valve for gas flow depending on the relative values of the inlet and outlet pressures (P_1 and P_2). In both cases the required valve flow capacity (C_v) is calculated given the flow rate through the valve and the pressure drop.

Critical (or Choked) Flow regime: Valid when ($P_1 \geq 2P_2$).

$$C_v = Q \frac{\sqrt{S.G. T}}{816 P_1}$$

where:

- ▪ ▪ Q is the gas flow rate (in Standard Cubic Feet per Hour)
- ▪ ▪ P_1 is the inlet pressure (in psi)
- ▪ ▪ P_2 is the outlet pressure (in psi)
- ▪ ▪ T is the absolute temperature in degrees R.
- ▪ ▪ S.G. is the specific gravity of medium, relative to air at 70 F and 14.7 psia (where S.G. is 1.0).
- ▪ ▪ C_v is the flow capacity of the valve. 1 C_v unit corresponds to 1 GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi.

Subcritical Flow regime: Valid when ($P_1 < 2P_2$).

$$C_v = \frac{Q}{962} \sqrt{\frac{(S.G. T)}{(P_1^2 - P_2^2)}}$$

where:

- ▪ ▪ Q is the gas flow rate (in Standard Cubic Feet per Hour)
- ▪ ▪ P_1 is the inlet pressure (in psi)
- ▪ ▪ P_2 is the outlet pressure (in psi)
- ▪ ▪ T is the absolute temperature in degrees R.
- ▪ ▪ S.G. is the specific gravity of medium, relative to air at 70 F and 14.7 psia (where S.G. is 1.0).
- ▪ ▪ C_v is the flow capacity of the valve. 1 C_v unit corresponds to 1 GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi.

Note that most manufacturers provide valve data (C_v vs. Diameter) in the American units system. The system does all appropriate conversions to display all variables in SI, except for the flow capacity, which is displayed in the above units (" C_v ").

In Design Mode the user specifies the pressure drop and maximum diameter. A manufacturer chart, relating C_v and Diameter is used to calculate the diameter. If the diameter exceeds the maximum the system assumes multiple units operating in parallel with a total Flow Capacity (C_v) equal to the calculated.

In Rating Mode, the user specifies the diameter and number of units. The system uses the manufacturer's chart to get the flow capacity and the resulting pressure drop.

[As the C_v vs. Diameter data may vary from manufacturer to manufacturer, the user can use the calculated Flow Capacity (C_v) for obtaining the exact diameter from any manufacturer chart.]

Pressure Drop Operation (Globe / Butterfly Valve - Gas)

This operation models the pressure drop of gases flowing through a control valve (globe or butterfly). The model described below is valid for small pressure drops in gas flow. The flow capacity formula, for calculating the C_v of a valve was design for liquid flow and is expressed in "GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi". However this flow capacity (in the same units) and similar formula is used for gas flow through a valve.

Equipment Sizing

Two different pressure regimes are considered for the sizing a valve for gas flow depending on the relative values of the inlet and outlet pressures (P_1 and P_2). In both cases the required valve flow capacity (C_v) is calculated given the flow rate through the valve and the pressure drop.

Critical (or Choked) Flow regime: Valid when ($P_1 \geq 2P_2$).

$$C_v = Q \frac{\sqrt{S.G. \cdot T}}{816 P_1}$$

where:

- ▪ ▪ Q is the gas flow rate (in Standard Cubic Feet per Hour)
- ▪ ▪ P_1 is the inlet pressure (in psi)
- ▪ ▪ P_2 is the outlet pressure (in psi)
- ▪ ▪ T is the absolute temperature in degrees R.
- ▪ ▪ S.G. is the specific gravity of medium, relative to air at 70 F and 14.7 psia (where S.G. is 1.0).
- ▪ ▪ C_v is the flow capacity of the valve. 1 C_v unit corresponds to 1 GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi.

Subcritical Flow regime: Valid when ($P_1 < 2P_2$).

$$C_v = \frac{Q}{962} \sqrt{\frac{(S.G. \cdot T)}{(P_1^2 - P_2^2)}}$$

where:

- ▪ ▪ Q is the gas flow rate (in Standard Cubic Feet per Hour)
- ▪ ▪ P_1 is the inlet pressure (in psi)
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- ▪ ▪ C_v is the flow capacity of the valve. 1 C_v unit corresponds to 1 GPM of water (at 60 F – S.G. =1) flowing with pressure drop of 1 psi.

Note that most manufacturers provide valve data (C_v vs. Diameter) in the American units system. The system does all appropriate conversions to display all variables in SI, except for the flow capacity, which is displayed in the above units (" C_v ").

The fully open valve flow capacity C_{vmax} is then calculated from the % opening:

$$C_{vmax} = C_v / (\% \text{ open}).$$

In Design Mode the user specifies the pressure drop and maximum diameter. A manufacturer chart, relating C_{vmax} and Diameter is used to calculate the diameter. If the calculated diameter exceeds the maximum specified, the system assumes multiple units operating in parallel with a total Flow Capacity (C_{vmax}) equal to the calculated.

In Rating Mode, the user specifies the diameter and number of units. The system uses the manufacturer's chart to get the flow capacity and the resulting pressure drop.

[As the C_{vmax} vs. Diameter data may vary from manufacturer to manufacturer, the user can use the calculated Flow Capacity (C_{vmax}) for obtaining the exact diameter from any manufacturer chart.]

Generic Box Operations

Load and Split Operation

It can be used to represent operations that combine supply of materials with simultaneous removal of selected components.

Material Supply (loading):

The supply of material can be done in 3 ways:

- (a) Amount of material to be loaded available in Input Stream
- (b) User specified mass of material to be loaded
- (c) User specified volume of material to be loaded

For the first case the loading of material, occurs as in the **Charge** or **Transfer In** operations depending on whether the selected stream is an input or an intermediate stream. For cases (b) and (c) the required flow of the pull-in stream is propagated backwards, through the network of connectivity.

Material Separation:

Component removal can also be specified by the user. The user can chose one or two output streams to which material will be separated and specify the percentage of each component that will be split in to that stream. For more details see the Separation Tab (Interface).

Duration:

If the duration of this operation is matched up to another operation (master operation), then the setup time, process time and turnaround time are simply derived from the master operation.

Pass-Through

The outlet stream is identical to the input stream.

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Equipment Purchase Cost

No default purchase cost model exists. To specify a value, right-click on the icon of the unit and select **Equipment Cost**. The dialog that is displayed allows you to specify a fixed cost or a function in a power-law format.

Operating Cost

To specify auxiliary utilities and labor parameters, right-click on the icon of the unit and select **Operating Cost Adjustments**.

Stoichiometric Reaction / Separation (in a GBX)

This is a multi-task operation which can be used to simulate continuous stoichiometric reaction (in a GBX) followed by flow or component splitting. You can choose to perform reaction calculations and or separation calculations. If you don't select any of these calculations then the operation acts as a pass through operation. (The separation option is not available in the 1x1 Continuous Generic Box Reaction(Bulk) Procedure.

Reaction Calculations:

The feed flowrate is calculated by adding the feed flowrates of all input streams. The reaction operation can handle any number of sequential material transformations (reactions) that happen continuously in generic equipment and for which kinetic expressions are unknown or unimportant. For more details click on the material balances tab.

The operating throughput (per unit) is calculated by dividing the feed flowrate by the number of units.

Separation Calculations:

You can choose either component or flow splitting. The splitting is performed after the reactions. You can specify either the component splits (% flows) or the total flow split, and whether this specification refers to the top or bottom splits. If the component split option is chosen the flowrates of each component is split into the 2 output streams according to the specified split for each component. If the total flow option is chosen the total flow rate is split into the 2 output streams according to the total flow specification.

Equipment Sizing:

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

Pass Through (Discrete Flow)

This unit operation performs no composition transformations on discrete entities that are fed into the unit. It simply allows the discrete entities to pass through it. It can be useful in simulating processing steps that involve no physico-chemical transformation, yet they incur some cost (e.g. inspection, weighing, etc.).

Equipment Sizing

If the equipment size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Convert to Discrete

This unit operation converts bulk material into discrete entities. It can be useful in modeling certain product formulation and packaging operations (e.g., formation of chocolate bars from molten chocolate). The user specifies the properties of the discrete entity (name and bulk amount) and the system calculates the operating discrete throughput (in entities/min).

Equipment Sizing

If the Equipment Size option is in Design Mode and the operating throughput exceeds the Maximum Throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/parts-min). In the second case, the specific power requirement times the operating throughput yields the power consumption.

Convert to Bulk

This unit operation converts discrete entities into flow of bulk material. It can be useful in modeling raw material recycling operations (e.g., recycling of plastic and glass containers). Also, whenever there is a need to feed discrete entities into a unit that expects bulk flow (e.g., incineration), a discrete-to-bulk generic box or an equivalent unit (e.g., a grinder or shredder) must be used to convert the inlet flow.

Equipment Sizing

If the **equipment** size option is in Design Mode and the operating throughput exceeds the maximum throughput, then, the system assumes multiple, identical units operating in parallel with an operating throughput of less than the maximum. If the equipment size option is in Rating Mode and the operating throughput exceeds the rated throughput of the step (which is equal to the rated throughput of each unit times the number of units), a warning message is displayed advising the user to increase the number of units or reduce the operating throughput.

To account for electricity consumption, the user can either specify the power demand (in kW) or the specific power requirement (in kW/kg-h). In the second case, the specific power requirement times the operating throughput yields the power consumption.

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