# 3.0 Components and Mixtures

Chemical components are used to represent the flow and composition of material in streams. Mixtures are used to facilitate initialization of feed streams in cases where certain raw materials (e.g., buffers) are consumed as mixtures. Pro-Designer comes equipped with two component and mixture databanks which, starting with version 4.5, come in relational database format (Microsoft Access .mdb format). The Designer databank includes approximately 360 components and 40 mixtures. It is maintained and constantly updated by our staff at Intelligen but, unlike previous versions of Pro-Designer, it cannot be edited or modified by the user. The User databank is an expandable user-maintained databank that allows users to readily add and edit information for additional pure components and stock mixtures according to their needs. Pro-Designer also supports the DIPPR pure component databank in its relational database format developed and maintained at Brigham Young University. The BYU-DIPPR databank contains over 1600 pure components along with their physical and thermodynamic properties compiled from the technical literature.

# 3.1 Registering Pure Components

When describing a new design case, you must register all components that will appear anywhere in the flowsheet. It is not necessary to provide all this information in the very beginning, because the component list of a design case can be modified at any time. However, as good practice, it is recommended that you consider the components that will appear in your flowsheet and introduce most of them early on, as several of the processing step's initialization parameters depend on the list of components present in the flowsheet (e.g., component separation factors, reaction stoichiometric coefficients, etc.) Components can be registered through the dialog that appears when you select the **Tasks: Register / Edit Pure Components...** menu item from the main menu (Figure 3.1).

Components can either be imported from the program's component databanks or defined for the first time for the needs of the specific design case. As indicated before, there are currently up to three different databanks from which the user can draw components: the Designer databank, the User databank and the DIPPR databank. The contents of the selected component databank are shown in the list box at the left of the dialog (see Figure 3.1). The components in the databank are indexed and can be listed in one of four ways:

**Component Indices**

**a.** Name,

**b.** Trade Name (or IUPAC Name for DIPPR components),

**c.** Chemical Abstract Service (CAS) Number, or

**d.** Local Name (or CAS Name for DIPPR components).

The name index and the trade name indices can be up to 31 characters long; the CAS

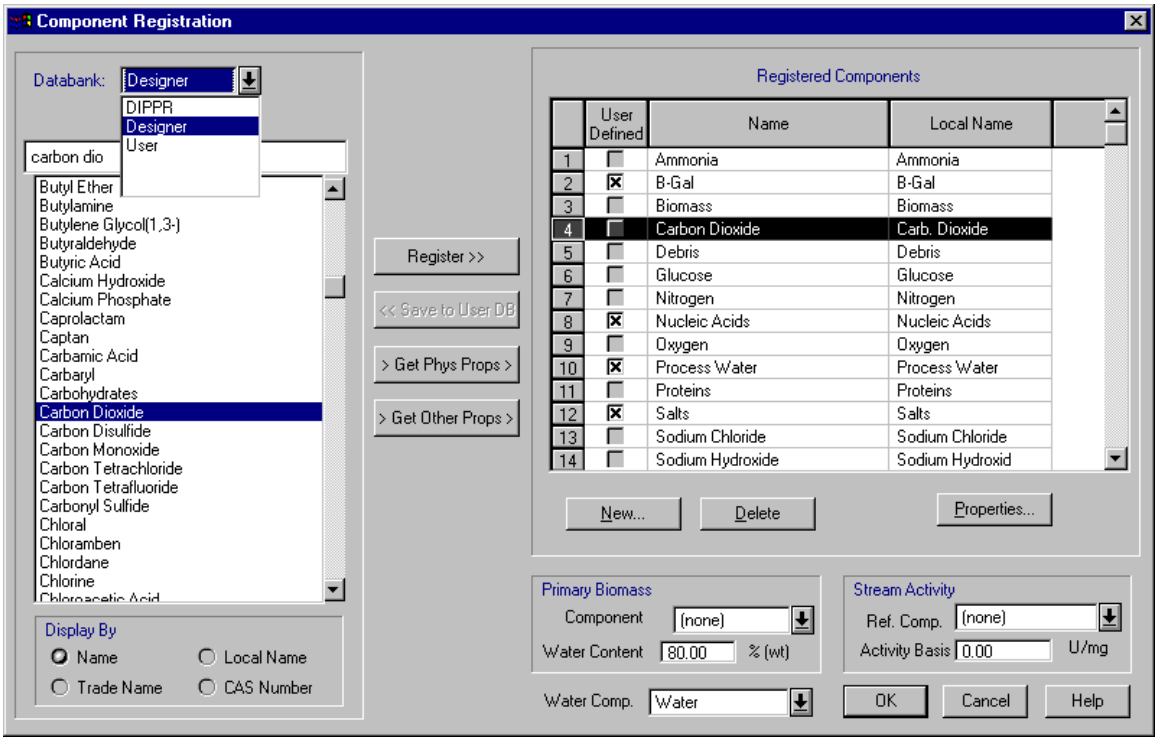


Figure 3.1: Pure component registration dialog.

number and the local name can be up to 15 characters long. Some chemicals in the Designer databank for which no CAS numbers could be found, are given made-up CAS numbers that are very easy to recognize: “N/A xxxx”. Local names are shorter versions of the full name of a chemical or they can be aliases by which a chemical is known to the members of your organization. The local name is the name by which a chemical registered in a design case will identify itself to the user in i/o dialogs of process steps and streams, reports, etc. and thus it becomes the ‘ID-Tag’ by which the given component is known to the system. Therefore, the system will not allow you to have in the same design case two components with the same local name.

## Caution!

Even though it is perfectly OK to have the same component (e.g. water) present in a design case under more than one local names (e.g. Process Water, WFI, USP Water) you should try to refrain from using the same local name for different components (e.g. water and hydrochloric acid) in your designs. Here is why this is a bad idea. Suppose you do use the same local name (say X) in two different design cases: in the first design case for water and in the second design case for hydrochloric acid. Suppose now, you decide to copy a process step from the first design case to the second. If the process step contains any component-related specifications (e.g. a set of separation coefficients, including X’s - for water) pasting the step to the destination design case will carry with it the specification but now, it will refer to a totally different component (hydrochloric acid).

### ➔ To Introduce a Chemical in the Current Design Case by Importing it from a Databank...

1. Select the desired databank. From the databank contents list box, select the chemical that you want to introduce in the design case. If the name (or CAS number) is not visible, you may scroll up or down until you locate it, or start typing the name at the top of the list box. Notice that as you type the program responds by automatically scrolling in order to bring the first entry that matches the typed portion of the name (or CAS number) at the top of the visible list.
2. Click on the **>> Register >>** button. Notice that as soon as you do that, the number of rows in the registration table will expand by one (component order may change as components are listed alphabetically.)

Even though all chemicals in the component databank have values for their fundamental properties, once they are introduced in a design case, these values can be overwritten. If you do that, then the new values will stay modified *only for that design case*. You don't have to provide values for all fundamental properties. Rather, you only need to provide values for the properties required by the simulation modules present in your design case. The usage of each fundamental property in each unit operation simulation module is provided later in this section. Here's how you edit the property values of registered components:

### ➔ To Edit the Fundamental Properties of a Single Component...

1. Locate the component in the registration table, and click on the box that displays the row number of the component (e.g., Number 4 for Carbon Dioxide in Figure 3.1). Notice that when you click on it, the whole row that describes the component is highlighted. Now the component is considered selected.
2. Click on the **Properties…** button and up comes a dialog with all the properties of the selected components organized in several groups (tabs). Each group of properties is described in detail in the next section

Sometimes you may need to introduce a component, which is not listed in the component databank, for the needs of your current design case. At this point, you have two options:

**(a)** Introduce the new component in the component databank (see below). Then import it in your own design case. That way, the component will always be available to be introduced in future design cases, if necessary.

**(b)** Introduce the new component in the current design case only (see next procedure). This option is useful if you don't have good values for all the properties of the component at this time, or if you don't think that any other design case may benefit from that component. Of course, if you change your mind later and decide to keep the component in the databank, you simply have to deposit it (see below.)

### ➔ To Introduce a New Chemical in the Current Design Case...

1. Click on **New...** (See Figure 3.1) and fill in the fields of the dialog that comes up (see Figure 3.2).

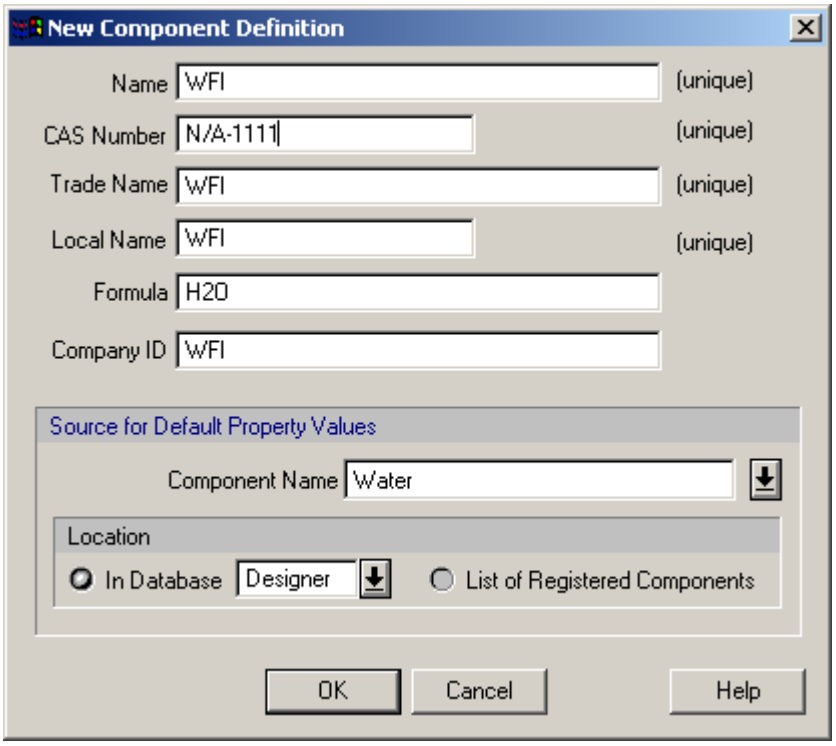


Figure 3.2: Definition of a new component.

Make sure you have typed the name of the component correctly. Once the component is introduced, this field cannot be edited again; the only way to modify it would be to completely remove it from the current design case and introduce it again under a new name. It is good practice to use unique (across the whole databank) strings for the name, trade name, CAS number and local name, in case you decide later to keep the component as a permanent member of the databank.

2. Select a *template component* that is already defined in one of the databanks or registered in the design case. The properties of the new component will be initialized to those of the selected template component.
3. Click on **OK**. Unless the program detects any conflicts in the definition of identification properties that need to be unique, the new component will be added to the list of registered components.

In all cases, the property values for the new component can always be edited as described in the previous paragraph. Even after initialization, it is still possible to copy the properties of one component into another or even the same component if that component happens to exist in more than one databanks but with different properties.

### ➔ To Copy the Properties of One Component into Another...

1. Invoke the component registration dialog (from the **Tasks: Register / Edit Pure Components...**).
2. From the Databank list box, select the databank where the template component (the one whose properties will be copied from) can be found. Select the component from the left-hand-side list.
3. From the table of registered components, select the desired component (whose properties are to be updated) by clicking on the button at the beginning of that component's row (e.g., Number 3 for Carbon Dioxide in Figure 3.1).
4. If you wish to copy only the physical and thermodynamic properties of the template component, click on the **>>Phys Props>>** button. By doing that, the format as well as the values of physical properties of the registered component will be changed to match the corresponding properties of the template component. If you wish to copy all other properties (aqueous, environmental and economic) of the template component, click on the **>>Other Props>>** button. Notice that this option is not available if the template component resides in the DIPPR databank because this databank does not provide such properties.

The use of the **>>Phys Props>>** and **>>Other Props>>** buttons as described above allows the mixing and matching of component properties from different sources without requiring explicit editing. This is also a convenient way to refresh the properties of components in old design cases without having to delete them and re-introduce them from the databank of choice. If after tailoring the properties of a component in a design case you wish to make this component available to other design cases, you must explicitly update the User databank as follows.

### ➔ To Deposit a Component of the Current Design Case into the User Component Databank...

1. Invoke the component registration dialog (from the **Tasks: Register / Edit Pure Components...**).
2. From the Databank list box, select the User databank.
3. Select the desired component in the table of registered components by clicking on the button at the beginning of that component's row (e.g., Number 3 for Carbon Dioxide in Figure 3.1).
4. Now, click on the **<< Deposit <<** button. If the component already exists in the databank, the program will request a further confirmation that indeed the intention is to update the component properties in the databank. Once you confirm that, the component databank will copy the component with the new component property values. In any future project that you may need to import that component from the User databank, the component will have the newly assigned set of values.

As mentioned before, new components can be introduced either in the User databank or in the current design case. If a component is introduced to the databank, then it will stay there and it can be retrieved for another design case. If the component is introduced to the design case, then it will only exist for the needs of that design case.

➔ **To Introduce a New Component in the User Databank...**

1. Open the databank component dialog by selecting the **Databank/Pure Components...** option of the menu (or hit **F2** as a shortcut.)
2. From the databank list box, select the User databank.
3. Click on **New...** and fill in the fields for the new component's name, CAS number, trade name, formula and local name (in a dialog similar to that of Figure 3.2.) Make sure you have typed the name of the component correctly. Once the component is introduced, this field cannot be edited again; the only way to modify it would be to completely delete it from the databank and introduce it again under a new name. All fields (except the formula) must contain strings that are unique across the whole databank. The system will not allow you to introduce a chemical that presents any index conflict with existing chemicals in the databank.

# 3.2 Fundamental Component Properties

Each component is identified in a design case by a local name, which is a user-definable identification tag. This local component name can be up to 15 characters long and is used as a short-cut reference of the component in streams' composition tables, process steps' simulation i/o dialogs, and reports.

For simulation, the program needs to know the fundamental properties of each component (such as, density, heat capacity, molecular weight, normal boiling point, compressibility factor, Antoine constants, etc.). These properties are called **fundamental** because all other properties (**derived**) are calculated (when required for simulation) based on the values of these properties. The fundamental properties are listed below. You should make every effort to provide the program with as accurate values of fundamental component properties as possible as this will affect strongly the accuracy of the simulation results. Note, however, that each component's property is employed in certain unit operation models only. Therefore, you don't need to provide accurate values for component properties that are not needed by the simulation of the processing steps in your current design case. That is why, in the list that follows, we mention the unit operations that require the corresponding property.

**Caution!**

Oftentimes users provide accurate values only for the minimum properties required for the current state of their design case and later, as the process is extended or modified and more processing steps are included, they neglect to revisit the component property dialogs and update the component properties. As each new component introduced in the design case (not imported from our component databank) is automatically assumed to have the properties of water, this may result in significant errors in the simulation and costing of your process.

The fundamental component properties are separated into six groups:

- **IDs**, and
- **Constant Physical Properties**, and

- **Temperature-dependent Physical Properties**, and
- **Aqueous Properties**, and
- **Economic Properties**, and
- **Pollutant Categorization.**

The aqueous group of component properties is related with the estimation of the environmental properties of streams (environmental impact assessment) and the modeling of unit operations typically found in waste treatment and pollution reduction processes. The pollutant categorization group of properties is related to the classification of a component as one of several classes of pollutants monitored by the EPA. For design cases where none of these issues is relevant, you may choose to ignore them.

## *Pure Component Properties: IDs*

- *Name*
  The formal name of a pure component. It was supplied when the component was originally introduced either to this design case or the databank, and cannot be edited. It can be a string of up to 31 characters.
- *Trade Name*
  The trade name of a pure component. It is supposed to display a name by which this component is widely known in the open market. It was given when the component was originally introduced either to this design case or the databank, but can be changed later. However it must be unique. It can be a string of up to 31 characters.
- *Formula*
  The formula of a pure component. It was given when the component was originally introduced either to this design case or the databank, but can be changed later. Uniqueness is not required. It can be a string of up to 31 characters.
- *Chemical Abstract Serial Number (CAS Number)*
  The CAS of the pure component (if available). It was given when the component was originally introduced either to this design case or the databank, but can be changed later. Uniqueness is required. It can be a string of up to 31 characters. For those components whose CAS number is not available (e.g. for all ‘pseudo-components’ like debris, biomass, etc.) the assigned number (string) is always by convention started with the characters “N/A,” and then followed by a number.
- *Company ID*
  Often components are identified and tracked within large corporations with their own tag ID number. This field is reserved to contain exactly that description. It was given when the component was originally introduced either to this design case or the databank, but can be changed later. Uniqueness is not required. It can be a string of up to 31 characters.
- *Is Biomass*
  A simple TRUE/FALSE flag that identifies component that can be treated as a biomass. Used in the designation of the primary biomass component and in all biological reactors.

- *Local Name*
  The local name is edible only when you first introduce a new component to the flowsheet.

## *Pure Component Properties: Constant Physical Properties*

- *Molecular Weight*
  Used in distillation, flash drum, condenser, absorber, and stripper, electrostatic precipitator, and all reactors.
- *Enthalpy of Formation* [J/gmol]
  Not used in the current version of the program.
- *Normal Boiling Point* [°C]
  Used in distillation, flash drum, and condenser. It is also used to determine the phase of a component (gas vs. liquid/solid). This is how the program decides whether to use the user-supplied correlation for density (applicable for liquid/solid phase) or use ideal gas law to determine the density (making the ideal gas assumption).
- *Normal Freezing Point* [°C]
  Used to determine if a given component is in liquid or solid form.
- *Critical Temperature* [K]
  Used in distillation, flash evaporation, and condensation.
- *Critical Pressure*[bar]
  Used in distillation, flash evaporation, and condensation.
- *Compressibility Factor*
  Used in distillation, flash evaporation, and condensation.
- *Acentric Factor (Omega)*
  Used in flash evaporation and condensation when an equation of state is selected.
- *Henry's Law Constant* [atm-$m^3$/mol]
  Used in absorption/stripping and VOC emission calculations.
- *Particle Size* [microns]
  Used in filters and centrifuges.
- *Default Volumetric Coefficient*
  Used in estimating the density of a stream (mixture of components) when this component participates in the composition of the stream.

## *Pure Component Properties: T-dependent Physical Properties*

- *Density* [kg/$m^3$ ]]
  Used in converting between mass and volumetric flowrates, and calculating the concentration of species in streams. For Pro-Designer-formatted components, the density correlation is assumed to apply for either the liquid or the solid phase (whichever applicable). If the system needs the density of a component in a vapor phase (i.e., at a temperature T that is higher than its normal boiling point) the system uses the ideal gas law or a user-selected equation of state to estimate the molar volume; then the density is taken as the inverse of the molar volume at that temperature (T).
- *Liquid/Solid Heat Capacity* [J/gmol-K]
  Used in energy balances.
- *Vapor Heat Capacity* [J/gmol-K]
  Used in energy balances.
- *Vapor Pressure* [mm Hg]
  Used in flash evaporation, and condensation.
- *Heat of Vaporization* [J/gmol]
  Used in energy balances in flash evaporation and condensation. The user can either provide the values of the correlation parameters or those parameters can be calculated from a combination of the Chen method for estimating the heat of vaporization at normal boiling point and of the Watson empirical formula for capturing the dependence on temperature (see 'The Properties of Gases and Liquids' by R.C. Reid, J.M. Prausnitz and B.E. Poling for details). The fundamental properties needed in these empirical formulas are the normal boiling point and the critical temperature and pressure.

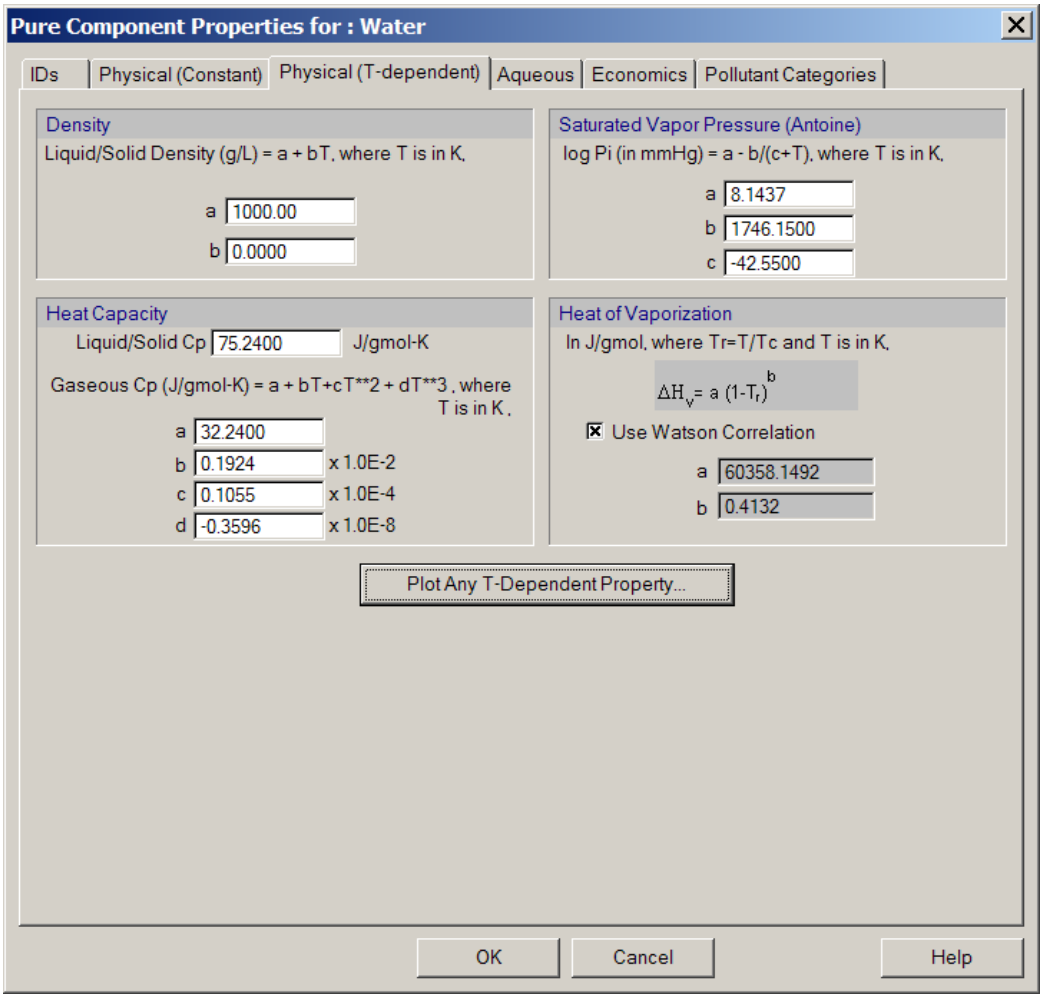


Figure 3.3: Temperature-dependent physical properties tab for a Pro-Designer formatted component.

The corresponding equations for Pro-Designer and DIPPR-formatted components are shown in Figures 3.3 and 3.4 respectively. There is a single equation for every property for Pro-Designer formatted components. DIPPR, on the other hand, offers up to 8 different equations shown in the right hand side of Figure 3.4. The selected equation is displayed in red color. The user can change the equation and edit the parameter values of DIPPR components that originate in the databank by selecting the **User-defined** radio button at the bottom left-hand side of the dialog. The user should be warned, however, that if those fields are edited, the original databank values are lost. The only way to recover them is to copy them from the original databank component. By pressing the **Plot Any T-Dependent Property** button the user is present with a dialog for choosing a physical property to be plotted as a function of temperature over a selected temperature range.

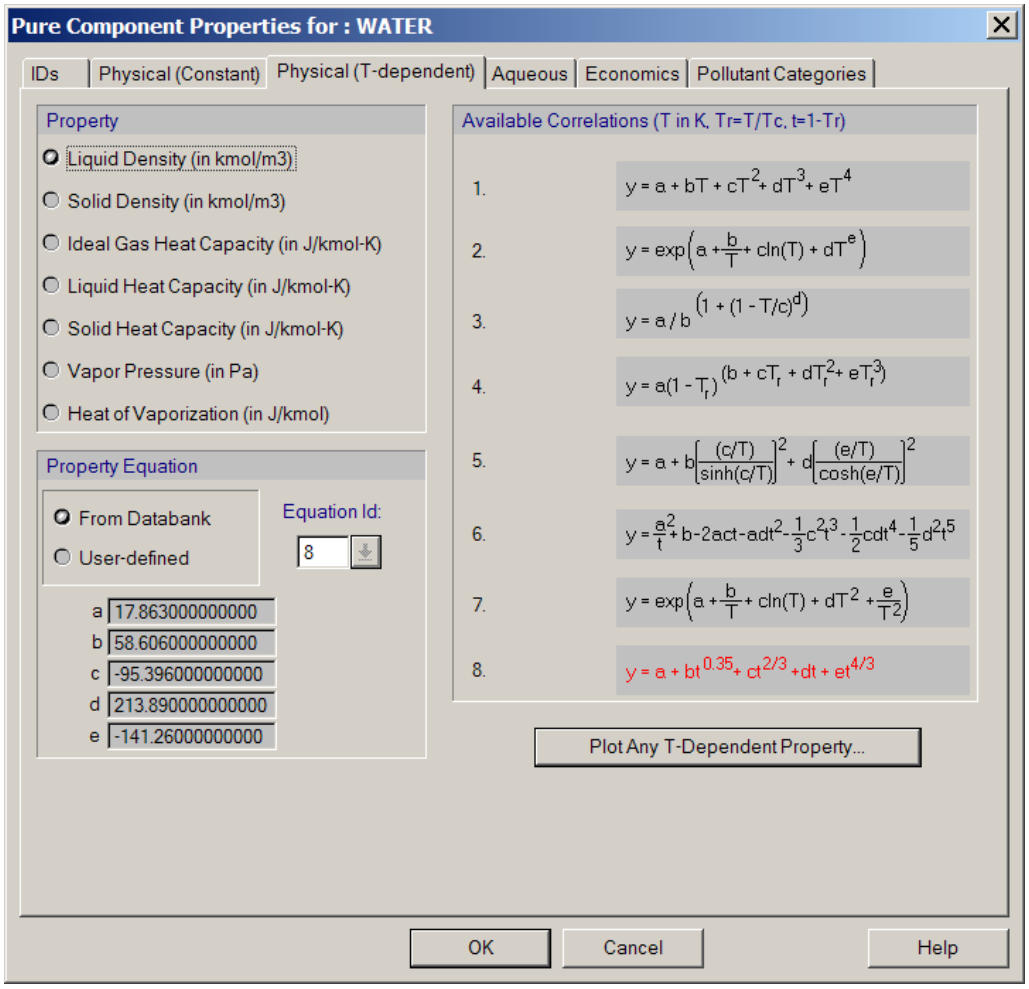


Figure 3.4: Temperature-dependent physical properties tab for a DIPPR-formatted component.

## *Pure Component Properties: Aqueous*

### Diffusivity Properties

- *Diffusivity in Water* [$cm^2/s$]
  Used in VOC emission calculations.

- *Diffusivity in Air* [$cm^2/s$]
  Used in VOC emission calculations.

**Bio-Degradation Properties**

- *Kmax* [mg substrate / g-biomass-h]
  Maximum biodegradation rate constant. Used in biodegradation reaction rate calculations in the Aerobic BioOxidation.
- *Ks* [mg/L]
  Half-saturation constant. Used in biodegradation reaction rate calculations in the Aerobic BioOxidation.

**Oxygen Ratios**

- *Chemical Oxygen Demand (COD)* [g oxygen / g substance]
  It represents the amount of oxygen (in g) required to chemically oxidize 1 g of the substance. It is used in calculating the COD value of material streams.
- *Theoretical Oxygen Demand (ThOD)* [g oxygen / g substance]
  It represents the theoretical amount of oxygen (in g) required for complete oxidation of 1g of the substance. It is usually equal to COD and is used in calculating the ThOD value of material streams.
- *BODu/COD*
  It represents the ratio of the ultimate biochemical oxygen demand (BODu) to the COD of a substance. It is used in calculating the BODu value of material streams based on the COD value of each component.
- *BOD5/BODu*
  It represents the ratio of the five-day BOD to ultimate BOD. It is used in calculating the BOD5 value of material streams based on the BODu values.

**Nitrogen Ratios**

- *Total Kjeldahl Nitrogen (TKN)* [g TKN / g substance]
  It represents the contribution of a component to total Kjeldahl nitrogen. It is used in calculating the TKN value of material streams.
- *Ammonia Nitrogen (NH3)* [g NH3 - N / g substance]
  It represents the contribution of a component to ammonia nitrogen. It is used in calculating the NH3 value of material streams.
- *Nitrate/Nitrite Nitrogen (NO3/NO2)* [g NO3/NO2 - N / g substance]
  It represents the contribution of a component to nitrate/nitrite nitrogen. It is used in calculating the NO3/NO2 value of material streams.

**Solid Ratios**

- *IsSolid* [Boolean]
  If TRUE, it indicates that this component is dissolved or suspended solid.
- *Total Solids (TS)* [g solids / g substance]
  It represents the fraction of a component that is dissolved or suspended solid (it will usually be either 0 or 1). It is used in calculating the TS value of material streams.
- *Total Suspended Solids (TSS / TS)* [g TSS / g TS]
  It represents the fraction of a solid component that is in suspension. It is used in

calculating the TSS value of material streams. Naturally, 1.0 - TSS represents the dissolved fraction of the component.

- *Volatile Suspended Solids (VSS / TSS)* [g VSS / g TSS]
  It represents the fraction of the suspended amount of a solid component that is volatile. It is measured as the organic fraction that oxidizes at 550 ±50 °C and is driven off as gas. It is used in calculating the VSS value of material streams.
- *Degradable Volatile Suspended Solids (DVSS / VSS)* [g DVSS / g VSS]
  It represents the fraction of the volatile suspended solid amount of a component that is biodegradable. It is used in calculating the DVSS value of material streams.
- *Volatile Dissolved Solids (VDS / TDS)* [g VDS / g TDS]
  It represents the fraction of the dissolved solid amount of a component that is volatile.
  It is used in calculating the VDS value of material streams.
- *Degradable Volatile Dissolved Solids (DVDS / VDS)* [g DVDS / g VDS]
  It represents the fraction of the volatile dissolved solid amount of a component that is biodegradable. It is used in calculating the DVDS value of material streams.

**Other**

- *Log10 (Octanol/Water)*
  The logarithm of the ratio of the concentrations of a component in octanol and water respectively. It indicates the hydrophobicity of a component and its tendency to associate with sludge. It is not used in the current version of the program.
- *Total Organic Carbon (TOC)* [g organic carbon / g substance]
  It represents the contribution of a component to organic carbon. It is used in calculating the TOC value of streams.
- *Total Phosphorous (TP)* [g phosphorous / g substance]
  It represents the contribution of a component to total phosphorous. It is used in calculating the TP value of streams.
- *CaCO3 Ratio* [g CaCO3 / g substance]
  It represents the contribution of a component to total CaCO3. It is used in calculating the CaCO3 value of streams.

## *Pure Component Properties: Economic*

- *Selling Price* [[$/kg]
  Used in economic calculations.
- *Purchasing Price* [[$/kg]
  Used in economic calculations.
- *Waste Treatment / Disposal Cost* [[$/kg]
  Used to estimate the waste treatment/disposal cost of a waste stream based on its composition; if you do not provide a direct cost for waste treatment/disposal of the entire stream on a per-kg-mixture-basis, a cost is estimated based on the contribution to the cost of each component present.
- *Supplier Name*
  Not used by the current version, useful only for reference by the users.

## *Pure Component Properties: Pollutant Categorization*

- *Is Hazardous* [Boolean]
  If TRUE, tags that component as hazardous. The presence of a hazardous component at a level higher than the hazardous threshold (see below) automatically tags the whole stream as hazardous.
- *Hazardous Threshold* [PPM]
  Designates the concentration level above which the component renders a whole stream as hazardous.
- *SARA 313* [Boolean]
  If TRUE, indicates that the component is included in a SARA-313 Chemicals section of the environmental impact report (EIR report).
- *33/50* [Boolean]
  If TRUE, indicates that the component is in the 33/50 EPA program and as such it will be included in the 33/50 Chemicals section of the EIR report.
- *Is Tracked in Solid Waste Streams* [Boolean]
  If TRUE, indicates that the component must be tracked in all solid waste streams and as such it will be present in the solid waste section of the EIR report.
- *Is Tracked in Aqueous Waste Streams* [Boolean]
  If TRUE, indicates that the component must be tracked in all aqueous waste streams and as such it will be present in the aqueous waste section of the EIR report.
- *Is Tracked in Organic Waste Streams* [Boolean]
  If TRUE, indicates that the component must be tracked in all organic waste streams and as such it will be present in the organic waste section of the EIR report.
- *Is Tracked in Emissions* [Boolean]
  If TRUE, indicates that the component must be tracked in all emissions and as such it will be present in the emissions section of the EIR report.

**Component Pollutant Primary Category:** One of: None (unregulated), VOC, Particulate, Acid Gas, ETG, CO, NOx, SO2, Base, or any of the user-defined categories

If a component is designated anything other than ‘None’, it will be included in the tallying up of the corresponding primary pollutant category as shown in the emissions section of the EIR report. Note that if the user has defined his/her own categories of pollutants (see Emission Limits Dialog ) then these categories will appear as well under the ‘Other’ group of categories.

**Components designated as VOCs**
If a component is designated as a VOC then it must be further categorized as follows: If it cannot be identified as belonging to any of the supplied 4 sub-categories (VCM, TVOS, EVOS or HAP-VOC), then it must be simply checked as ‘other’ VOC. Limits for all above subcategories are specified by the EPA.

**Components designated as Particulates**

If a component is designated as a particulate then it must be further categorized as follows: If it cannot be identified as belonging to any of the supplied 8 sub-categories (Biological, Radionucleid, Asbestos, Dioxin, LOC, HAP, Cr+6, Metal) then it must be simply checked as 'other' VOC. Limits for all above subcategories are specified by the EPA.

**Components designated as Acid Gases**
If a component is designated as a Acid Gas then it must be further categorized as either HAP-Acid gas or non-HAP Acid Gas.Limits for these subcategories are specified by the EPA.

**Component designated as ETGs**
If a component is designated as a ETG then it must be further categorized as either HAP-ETG or non-HAP ETG. Limits for these subcategories are specified by the EPA. For all of the above primary and secondary classifications of pollutants, you can specify the allowable limits and Pro-Designer will tally up the contributions from all emission streams of your process and will notify you if any violations occur against user-preset limits.

# 3.3 Pollutant Categories

The following tables should be used to categorize all raw materials and air pollutants into the appropriate category and sub-category. In some cases the material may appear in more than one category. For example, heavy organics with vapor pressures less than 1 mmHg cold be detected (depending on temperature) by NJ Air Test Method 3 as a hydrocarbon and/or by Method 1as a liquid particulate. The material would be placed in the Total VOC category (sub-category: OTHER VOC) as well as in category Total Particulate (sub-category: LOC). Also, an acid may appear in both the Total Particulate category as well as the Acid Gases category depending on whether or the acid combines with water to form liquid particulate. If it is known that a material would not fall into any other categories and sub-categories double-listing is not required. However, double-listing is recommended when there is uncertainty as to how the material will behave during a stack test. Pro-Designer does allow listing of materials into more than one categories.

Note that Pro-Designer allows you to define up to five more categories (user-defined pollutant categories) in case your state regulations require you to do so. You can define these extra categories (along with their regulated limits) by selecting **Preferences / Emission Limits…** from the flowsheet's context menu. See the following section (Sec 3.4) for more details.

| **CATEGORY I** | **Total Particulate**<br><br>All materials which could not be detected under NJ Air Test Method 1 | **Sub-Category** |
|---|---|---|

| | | |
|---|---|---|
| | A. Infectious agents which require practices, safe equipment and facilities that constitute Biosafety Level 2 or higher (see Note 2) | BIOLOGICAL |
| | B. Radionuclide as listed in N.J.A.C. 7:28-6.5 which are contained particulates | RADIONUCLIDE |
| | C. Compounds of hexavalent chromium which are particulates | Cr+6 |
| | D. Compounds of any of the following metals which are particulates: Pb, Hg, Cd, Be, As, Ni, Cr (total) | METAL |
| | E. Particulates which contain Asbestos | ASBESTOS |
| | F. DIOXINS (see Note 3) | DIOXIN |
| | G. Materials which are liquid organic compounds emitted as particulate | LOC |
| | H. Hazardous Air Pollutants listed in Note 10 | HAP-PARTICULATE |
| | I. Particulates which are not included in A-H | OTHER PARTICULATE |

| **CATEGORY II** | **Total VOC (Volatile Organic Compound)**<br><br>All materials which could not be detected under NJ Air Test Method 3 (see Note 6) | **Sub-Category** |
|---|---|---|
| | A. Vinyl Chloride Monomer | VCM |
| | B. Materials which are toxic volatile organic substances listed in NJAC 7:27-17 Table 1 | TVOS |
| | C. Materials which are exempt volatile organic substances listed in NJAC 7:27-16.1 (see Note 4) | EVOS |
| | D. Hazardous Air Pollutants listed in Note 10 except VCM | HAP-VOC |
| | E. Volatile Organic Compounds which are not included in A through D | OTHER VOC |

| CATEGORY III | **Acid Gases**<br><br>Materials that are acid gases and may not be detected as a particulate using NJ Air Test Method 1 or as VOC using Method 3 | **Sub-Category** |
|---|---|---|
| | A. Hazardous Air Pollutants listed in Note 8 | HAP-ACID |
| | B. Acid Gases which are not included in A. Includes, but is not limited to, $F_2$, $SO_3$ and $H_2S$ | ACID |

| CATEGORY IV | **Extraordinarily Toxic Gases (ETG)** | **Sub-Category** |
|---|---|---|
| | A. Hazardous Air Pollutants listed in Note 9 | HAP-GAS |
| | B. Gases which are listed in Note 5 | GAS |

| CATEGORY V | **CO** | **Sub-Category** |
|---|---|---|
| | Carbon Monoxide | CO |

| CATEGORY VI | **NOx** | **Sub-Category** |
|---|---|---|
| | Nitrogen Oxides: includes $N_2O$, NO, $N_2O_3$, $N_2O_4$, $NO_2$, $N_2O_5$, $N_3O_4$ and $NO_3$ (see Note 7) | NOx |

| CATEGORY VII | **$SO_2$** | **Sub-Category** |
|---|---|---|
| | Sulfur Dioxide | $SO_2$ |

| CATEGORY VIII | **Base Gases** | **Sub-Category** |
|---|---|---|
| | Materials which are base gases and may not be detected as a particulate using NJ Air Test Method 1 or as VOC using Method 3. Includes but is not limited to $NH_3$ | BASE |

**NOTES:**

1. All air pollutants and raw materials are characterized using these standardized categories. Materials which are not accurately described by the above categories and sub-categories may either be listed individually or be included under one of additional five user-defined categories that Pro-Designer allows you to introduce. This listing excludes distillates of air as defined in NJAC 7:27-8.1. The addition of categories and sub-categories after approval may require an alteration to the permit and certificate for the process.

2. This sub-category includes infectious agents requiring practices, safety equipment and facilities that constitute Biosafety Level 2 or higher. See HHS Publication No. (NIH 88-8395, 2nd Edition (May 1988)).

3. The Dioxin sub-category will include the following isomers of chlorinated dibenzo-p-dioxin (CDDs) and chlorinated dibenzofurans (CDFs):

| | |
|---|---|
| 2,3,7,8 – TCDD | 2,3,7,8 – TCDF |
| 1,2,3,7,8 – PeCDD | 1,2,3,7,8 – PeCDF |
| 1,2,3,4,7,8 – HxCDD | 2,3,4,7,8 – PeCDF |
| 1,2,3,7,8,9 – HxCDD | 1,2,3,4,7,8 – HxCDF |
| 1,2,3,6,7,8 – HxCDD | 1,2,3,7,8,9 – HxCDF |
| 1,2,3,4,6,7,8 – HpCDD | 1,2,3,6,7,8 – HxCDF |
| | 2,3,4,6,7,8 – HxCDF |
| | 1,2,3,4,6,7,8 – HpCDF |
| | 1,2,3,4,7,8,9 – HpCDF |

   Source: EPA 625/3-87/012,Interim Procedures for Estimating Risks Associated with Exposures to Mixtures of Chlorinated p- Dioxins and Dibenzofurans (CDDs and CDFs) p.11

4. Includes the following:

| | |
|---|---|
| Methane | |
| Trichlorofluoromethane | 1,1,2-Trichloro-1,2,2,-Trifluoroethane |
| Dichlorodifluoromethane | 1,2,-Dichloro-1,1,2,2 Tertafluoroethane |
| Chlorodifluoromethane | Chloropentafluoroethane |
| Trifluoromethane | |

5. Extraordinarily Toxic Gases are defined as the following chemicals:

| **Name** | **CAS Number** |
|---|---|
| Boron Trichloride ($BCl_3$) | 10294-34-5 |
| Boron Trifluoride ($BF_3$) | 7637-07-2 |
| Bromine Chloride (BrCl) | 13863-41-7 |
| Chlorine Dioxide ($ClO_2$) | 10049-04-4 |
| Chlorine Pentafluride ($ClF_5$) | 13637-63-3 |
| Chlorine Trifluoride ($ClF_3$) | 7790-91-2 |
| Diborane ($B_2H_6$) | 19287-45-7 |
| Dichlorosilane ($H_2Cl_2Si$) | 4109-96-0 |
| Hydrogen Selenide ($H_2Se$) | 7783-07-5 |

| | |
|---|---|
| Nitrogen Trifluoride ($NF_3$) | 7783-41-7 |
| Oxygen Difluoride ($OF_2$) | 7783-41-7 |
| Ozone ($O_3$) | 10028-15-6 |
| Perchloryl Fluoride ($ClFO_3$) | 7616-94-6 |
| Phosphorous Trifluoride ($PF_3$) | 7783-55-3 |
| Selenium Hexafluoride ($SeF_6$) | 7783-79-1 |
| Stibine ($SbH_3$) | 7803-52-3 |
| Sulfur Tetrafluoride ($SF_4$) | 7783-60-0 |
| Sulfuryl Fluoride ($SF_2O_2$) | 2699-79-8 |
| Tellurium Hexafluoride ($TeF_6$) | 7783-80-4 |
| Tetrafluorohydrazine ($N_2F_4$) | 10036-47-2 |

6. CO2 is NOT a VOC

7. Nitrogen Oxides are as follows: N2O (nitrous oxide), NO (nitric oxide), N2O4 (dinitrogen tetroxide or nitrogen peroxide), NO2 (nitrogen dioxide), N2O5 (dinitrogen pentoxide), N3O4 (trinitrogen tetroxide) and NO3 (nitrogen trioxide).

8. Includes the following chemicals:

| **Name** | **CAS Number** |
|---|---|
| Chlorine | 7782505 |
| Hydrogen Chloride | 7647010 |
| Hydrogen Fluoride | 7664393 |

9. Includes the following chemicals:

| **Name** | **CAS Number** |
|---|---|
| Phosphine ($PH_3$) | 7803-51-2 |
| Arsine ($AsH_3$) | 7784-42-1 |

10. Includes the following chemicals (from the Clean Air Act Amendments of 1990 list of Hazardous Air Pollutants):

| **Name** | **CAS Number** |
|---|---|
| Acetaldehyde | 75070 |
| Acetamide | 60355 |
| Acetonitrile | 75058 |
| Acetophenone | 98862 |
| 2-Acetylaminofluorene | 53963 |
| Acrolein | 107028 |
| Acrylamide | 79061 |
| Acrylic Acid | 79107 |
| Acrylonitrile | 107131 |
| Allyl chloride | 107051 |
| 4-Aminobiphenyl | 92671 |
| Aniline | 62533 |
| o-Anisidine | 90040 |
| Asbestos | 1332214 |

| | |
|---|---|
| Benzene (including benezene from gasoline) | 71432 |
| Benzidine | 92875 |
| Benzotrichloride | 98077 |
| Benzyl Chloride | 100447 |
| Biphenyl | 92524 |
| Bis (2-ethylhexyl) phthalate (DEHP) | 117817 |
| Bis (chloromethyl) ether | 542881 |
| Bromoform | 75252 |
| 1,3-Butadiene | 106990 |
| Calcium cyanamide | 156627 |
| Caprolactam | 105602 |
| Captan | 133062 |
| Carbaryl | 63252 |
| Carbon disulfide | 75150 |
| Carbon tetrachloride | 56235 |
| Carbonyl sulfide | 463581 |
| Catechol | 120809 |
| Chloramben | 133904 |
| Chlordane | 57749 |
| Chloroacetic acid | 79118 |
| 2-Chloroacetophenone | 532274 |
| Chlorobenzene | 108907 |
| Chlorobenzilate | 510156 |
| Chloroform | 67663 |
| Chloromethyl methyl ether | 107302 |
| Chloroprene | 126998 |
| Cresols/Cresylic acid (isomers and mixtures) | 1319773 |
| o-Cresol | 95487 |
| m-Cresol | 108394 |
| p-Cresol | 106445 |
| Cumene | 98828 |
| 2,4-D, salts and esters | 94757 |
| DDE | 3547044 |
| Diazomethane | 334883 |
| Dibenzofurans | 132649 |
| 1,2-Dibromo-3-chloropropane | 96128 |
| Dibutylphthalate | 84742 |
| 1,4-Dichlorobenzene(p) | 106467 |
| 3,3-Dichlorobenzidene | 91941 |
| Dichloroethyl ether (Bis(2-chloroethyl)ether) | 111444 |
| 1,3-Dichloropropene | 542756 |
| Dichlorovos | 62737 |
| Diethanolamine | 111422 |
| N,N-Diethyl aniline (N,N-Dimethylaniline) | 121697 |
| Diethyl Sulfate | 64675 |
| 3,3-Dimethoxybenzidine | 119904 |
| Dimethyl aminoazobenzene | 60117 |
| 3,3’ - Dimethyl benzidine | 119937 |
| Dimethyl carbomoyl chloride | 79447 |

| | |
|---|---|
| Dimethyl formamide | 68122 |
| 1,1-Dimethyl hydrazine | 57147 |
| Dimethyl phthalate | 131113 |
| Dimethyl sulfate | 77781 |
| 4,6-Dinitro-o-cresol, and salts | 534521 |
| 2,4-Dinitrophenol | 51285 |
| 2,4-Dinitrotoluene | 121142 |
| 1,4-Dioxane (1,4-Diethyleneoxide) | 123911 |
| 1,2-Diphenylhydrazine | 122667 |
| Epichlorohydrin (1-Chloro-2,3-epoxypropane) | 106898 |
| 1,2-Epoxybutane | 106887 |
| Ethyl acrylate | 140885 |
| Ethyl benzene | 100414 |
| Ethyl carbamate (Urethane) | 51796 |
| Ethyl chloride (Chloroethane) | 75003 |
| Ethylene dibromide (Dibromoethane) | 106934 |
| Ethylene dichloride (1,2-Dichloroethane) | 107062 |
| Ethylene glycol | 107211 |
| Ethylene imine (Aziridine) | 151564 |
| Ethylene oxide | 75218 |
| Ethylene thiourea | 96457 |
| Ethylidene dichloride (1,1-Dichloroethane) | 75343 |
| Formaldehyde | 50000 |
| Heptachlor | 76448 |
| Hexachlorobenzene | 118741 |
| Hexachlorobutadine | 87683 |
| Hexachlorocyclopentadine | 77474 |
| Hesachloroethane | 67721 |
| Hexamethylene-1,6-diisocyanate | 822060 |
| Hexamethylphosphoramide | 680319 |
| Hexane | 110543 |
| Hydrazine | 302012 |
| Hydrochloric acid | 7647010 |
| Hydrofluoric acid | 7664393 |
| Hydroquinone | 123319 |
| Isophorone | 78591 |
| Lindane (all isomers) | 58899 |
| Maleic anhydride | 108316 |
| Methanol | 67561 |
| Methoxchlor | 72435 |
| Methyl bromide (Bromomethane) | 74839 |
| Methylchloride (Chloromethane) | 74873 |
| Methyl chloroform (1,1,1-Trichloroethane) | 71556 |
| Methyl ethyl ketone (2-Butanone) | 78933 |
| Methyl hydrazine | 60344 |
| Methyl iodide (Iodomethane) | 74884 |
| Methyl isobutyl ketone (Hexone) | 108101 |
| Methyl isocyanate | 624839 |
| Methyl methacrylate | 80626 |

| | |
|---|---|
| Methyl tert butyl ether | 1634044 |
| 4,4-Methylene bis (2-chloroaniline) | 101144 |
| Methylene chloride (Dichloromethane) | 75092 |
| Methylene diphenyl disocyanate (MDI) | 101688 |
| 4,4’-Methylenedianiline | 101779 |
| Naphtalene | 91203 |
| Nitrobenzene | 98953 |
| 4-Nitrobiphenyl | 92933 |
| 4-Nitrophenol | 100027 |
| 2-Nitropropane | 79469 |
| N-Nitroso-N-methylurea | 684935 |
| N-Nitrosodimethylamine | 62759 |
| N-Nitrosomorpholine | 59892 |
| Parathion | 56382 |
| Pentachloronitrobenzene (Quintobenzene) | 82688 |
| Pentachlorophenol | 87865 |
| Phenol | 108952 |
| p-Phenylenediamine | 106503 |
| Phosgene | 75445 |
| Phosphorus | 7723140 |
| Phthalic anhydride | 85449 |
| Polychlorinated biphenyls (Aroclors) | 13336363 |
| 1,3-Propane sultone | 1120714 |
| beta-Propiolactone | 57578 |
| Propionaldehyde | 123386 |
| Propoxur (Baygon) | 114261 |
| Propylene dichloride (1,2-Dichloropropane) | 78875 |
| Propylene oxide | 75569 |
| 1,2-Propylenimine (2-Methylaziridine) | 75558 |
| Quinoline | 91225 |
| Quinone | 106514 |
| Styrene | 100425 |
| Styrene oxide | 96093 |
| 2,3,7,8-Tetrachlorodibenzo-p-dioxin | |
| 1,1,2,2-Tetrachloroethane | |
| Tetrachloroethylene (Percyoroethylene) | |
| Titanium tetrachloride | |
| Toluene | |
| 2,4-Toluene diamine | |
| 2,4-Toluene diisocyanate | |
| o-Toluidine | |
| Toxaphene (Chlorinate camphene) | |
| 1,2,4-Trichlorobenzene | |
| 1,1,2-Trichloroethane | |
| Trichloroethylene | |
| 2,4,5-Trichlorophenol | |
| 2,4,6-Trichlorophenol | |
| Triethylamine | |
| Trifluralin | |

| | |
|---|---|
| 2,2,4-Trimethylpentane | |
| Vinyl acetate | |
| Vinyl bromide | |
| Vinyl chloride | |
| Vinylidene chloride (1,1-Dichloroethylene) | |
| Xylenes (isomers and mixture) | |
| o-Xylenes | |
| m-xylenes | |
| p-xylenes | |
| Antimony Compounds | |
| Arsenic Compounds (inorganic) | |
| Beryllium Compounds | |
| Cadmium Compounds | |
| Chromium Compounds | |
| Cobalt Compounds | |
| Cyanide Compounds (see note a) | |
| Glycol ethers (see note b) | |
| Lead Compounds | |
| Manganese Compounds | |
| Mercury Compounds | |
| Nikel Compounds | |
| Polycyclic Organic Matter (see note c) | |
| Selenium Compounds | |

**Notes**: For all listings above which contain the word “compounds” and for glycol ethers, the following applies: Unless otherwise specified, these listings are defined as including any unique chemical substance that contains the names chemical (i.e. antimony, arsenic, etc.) as part of that chemicals infrastructure.

a. X’CN where X-H’ or any other group where a formal dissociation may occur. For example, KCN or Ca $(CN)_2$.

b. Includes mono- and di- ethers or ethylene glycol, diethylene glycol, and triethylene glycol R-(OCH2CH2)n-OR’ where:
n = 1,2 or 3
R = alkyl or aryl groups
R’ = R, H or groups which when removed yield glycol ethers with the structure R-(OCH2CH)n – OH.
Polymers are excluded from the glycol category.

c. Includes organic compounds with more than one benzene ring, and which have a boiling point greater or equal to 100 ºC.

# 3.4 User-Defined Pollutant Categories & Emission Limits

Even though the current pollutant categorization options are fairly extensive, Pro-Designer allows you define up to five extra user-defined categories of pollutants (which may be required by your local state regulations). Once you introduce these new

categories, they will appear as new options in the Pollutant Categories tab of every pure component introduced in your design case.

To introduce new user-defined pollutant categories you select **Preferences / Emission Limits…** from the flowsheet's context menu. Then the dialog of Fig. 3.5 appears.

From the same dialog you can also specify maximum allowable limits for each of the pollutant categories. Pro-Designer will tally up the contribution to each category from every emission stream associated with this process and will warn you if the total in any category exceeds the limits as specified from this dialog.

The emissions report presents a complete analysis and breakdown of emissions to all pollutant categories.

# 3.5 Special Components

Certain components in the set of registered components in a design case have a special meaning for the system's simulation engine. There are currently three such components:

**a.** ***The water component***: the component designated to represent the liquid form of water that is associated with the primary biomass component.

**b.** ***The primary biomass component***: the component assumed to represent the biomass (or sludge – for wastewater treatment applications) flow that the intracellular (or sorbed) portions of other components associate with. If primary biomass is formed (as a product of a bioreaction) and the water component has been identified (see above definition) the system will adjust automatically the intracellular water in order to satisfy the biomass water content as specified during component registration (see Figure 3.1). Furthermore, when the primary biomass component has been identified and, during a separation process, is assigned a removal coefficient, the system will use the same removal coefficient for the intracellular portion of all components. The primary

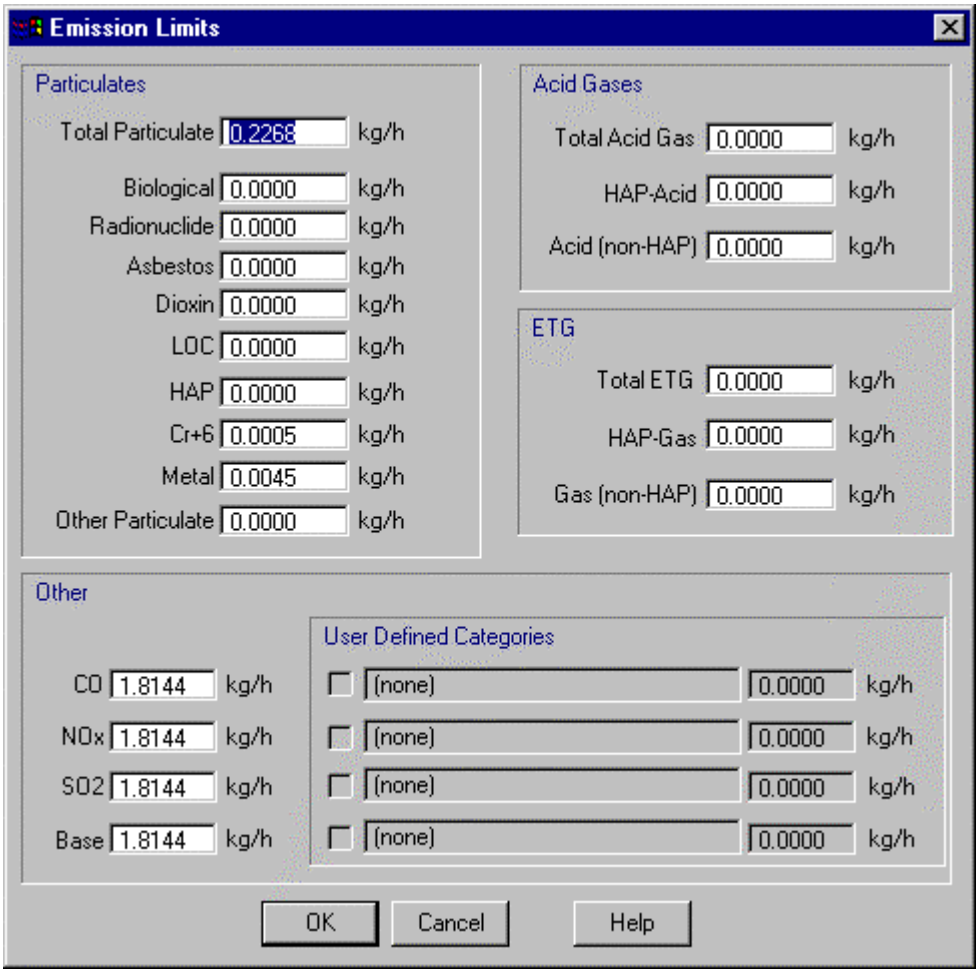


Figure 3.5: Emission Limits Dialog.

biomass component is selected among components whose "IsBiomass" flag has been set (i.e., declared as a biomass.)

c. ***The activity-reference component***: the component whose concentration is used to determine the activity strength of a stream. Of course, in order to do that calculation we also need the potency index of the active component. The potency index represents how many (arbitrary) units of activity (U) should be accounted for each mg of the active component present in a stream.

The special components are selected from the set of components registered in the current design through the component registration dialog (see previous section.) The primary biomass component must be a component whose 'IsBiomass' flag is turned on (only such components appear in the relevant selection list box of the component registration dialog).

Note that certain unit operation models may treat additional components in a unique way. In this case, specification of such components is done at that particular processing step and the scope of such a definition is also restricted within the limits of that process step only. Distillation columns, for example, require specification of the "heavy key" and the "light key" components. Specifying component X as the heavy key and Y as the light key in column D-1, does not imply that the same components will be used as

the heavy and light key components respectively in any other distillation column. Instead, you have to redefine them using the i/o dialog of each process step that requires such as a specification.

# 3.6 Registering Stock Mixtures

Mixtures facilitate initialization of feed streams in cases where certain raw materials (e.g., buffers, acid solutions, base solutions, etc.) are utilized as mixtures. Any information about mixtures is lost in intermediate and output streams. Pro-Designer converts mixture flowrates into their equivalent pure component flows and performs material balances and reports results based on pure component data.

Mixtures can be registered through the dialog that appears when you select the **Tasks: Register / Edit Stock Mixtures...** menu item from the main menu (Figure 3.6). The program also automatically registers all pure components that are ingredients of the mixture (a notification message makes the user aware of this action).

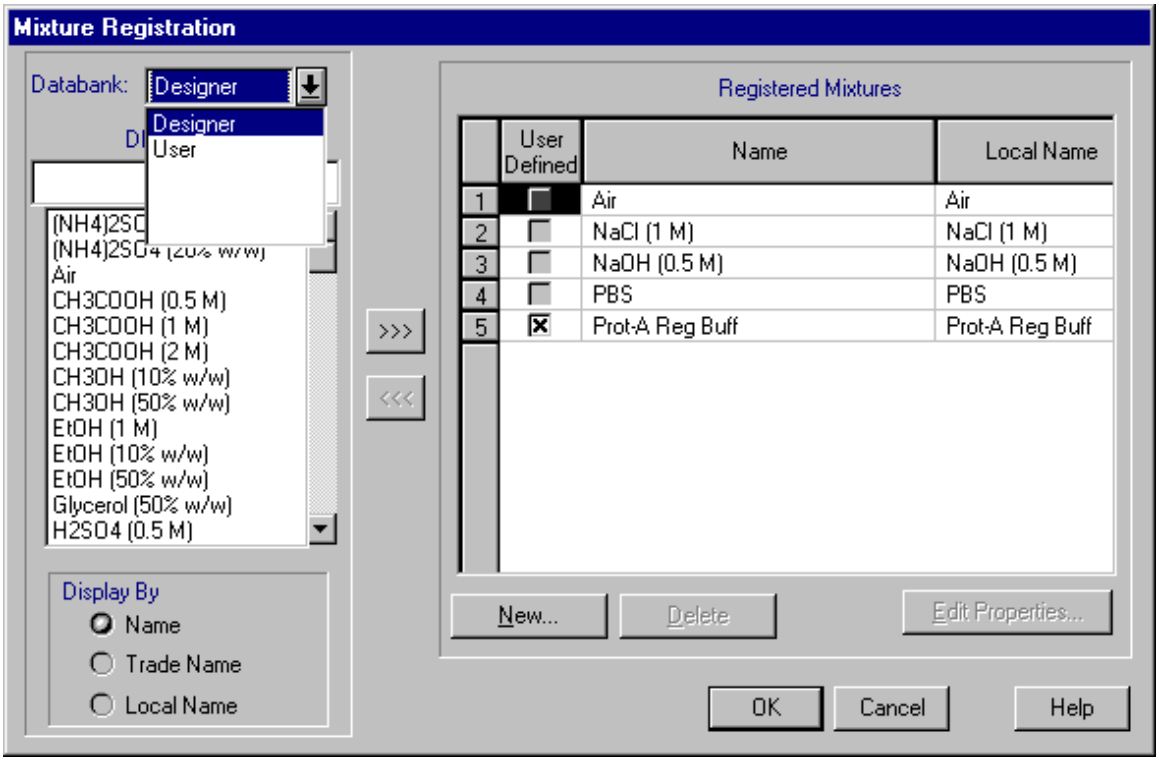


Figure 3.6: Stock mixture registration dialog.

Stock mixtures, like pure components, can either be imported from the program's mixture databanks or defined for the first time for the needs of the specific design case. The contents of the selected (Designer or User) mixture databank are shown in the list box at the left of the dialog (see Figure 3.6). The mixtures in the databank are indexed and can be listed based on Name, Trade Name, and Local Name.

### ➔ To Introduce a Mixture in the Current Design Case by Importing it from a Databank...

1. Select the desired databank. From the databank contents list box, select the mixture that you want to introduce in the design case. If the name is not visible, you may scroll up or down until you locate it or start typing the name at the top of the list box. Notice that as you type the program responds by automatically scrolling in order to bring the first entry that matches the typed portion of the name at the top of the visible list.
2. Click on the **>>>** button. Notice that as soon as you do that, the number of rows in the registration table will expand by one (mixture order may change as mixtures are listed alphabetically.)

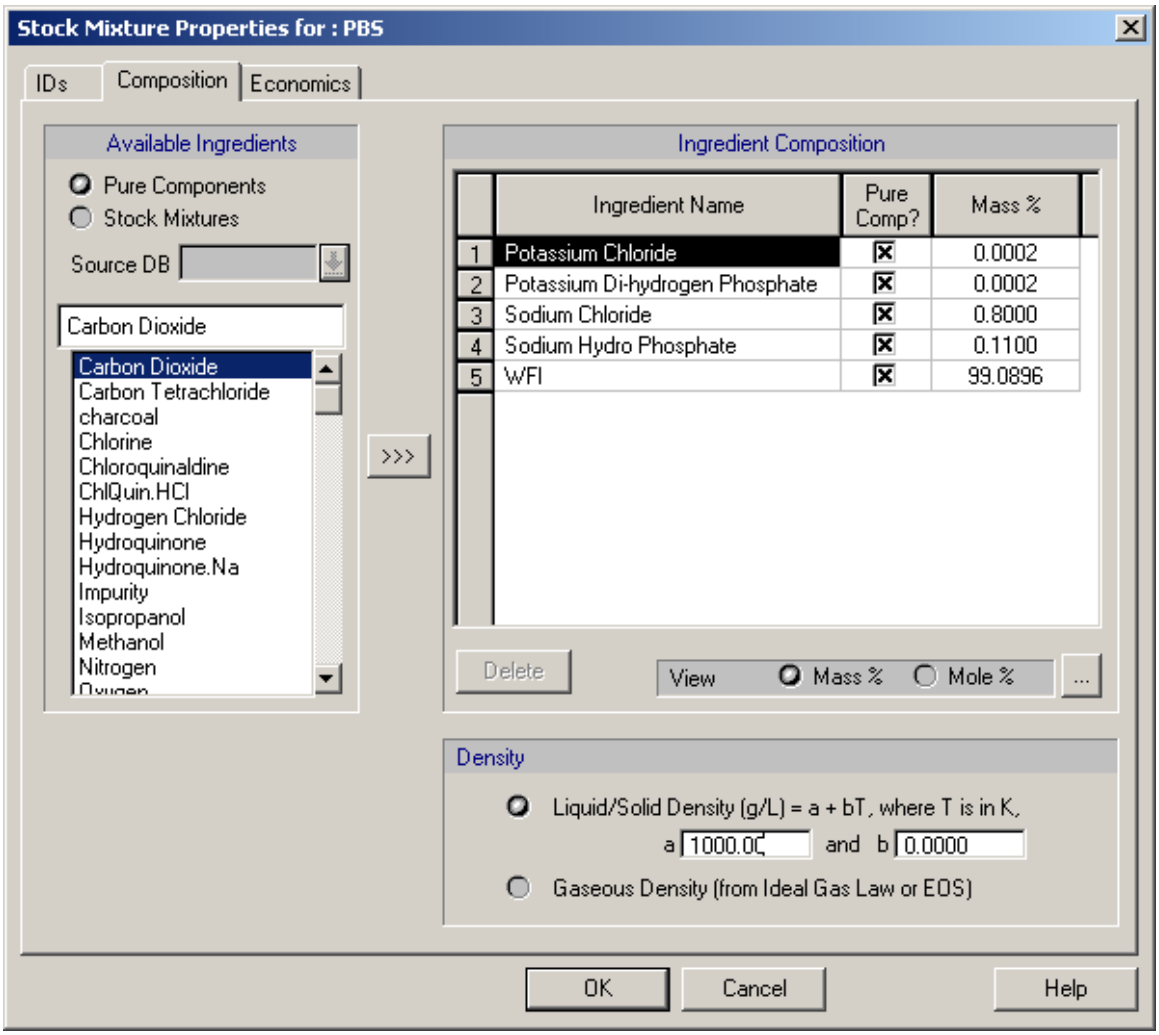


Figure 3.7: Dialog for editing the properties of a mixture.

➔ **To Edit the Fundamental Properties of a Stock Mixture...**

1. Locate the mixture in the registration table, and click on the box that displays the row number of the mixture (e.g., Number 4 for PBS in Figure 3.6). Notice that when you click on it, the whole row that describes the mixture is highlighted. Now the mixture is considered selected.
2. Click on **Properties…** to bring up the dialog of Figure 3.7 through which you view and edit the properties of the selected mixture.

➔ **To Introduce a New Mixture into the Current Design Case...**

Click on **New...** (See Figure 3.6) and fill in the fields of the dialog that comes up. Then, select the newly defined mixture and click on **Properties**… to specify the composition and other properties of the new mixture. To introduce a new mixture into the application mixture databank, select **Databanks / Stock Mixtures…** and follow the same procedure as if you introduced a new mixture into the design case.

# 3.7 Mixture Properties

The properties of a mixture are limited to its composition, density, and purchase price.

- *Composition*
  The composition of a mixture is defined on a mass or mole basis. A mixture can be composed of pure components as well as of other mixtures.

- *Density* [g/L or kg/$m^3$ ]
  Used in converting between mass and volumetric flowrates, and calculating the concentration of species in streams. The density is assumed to apply for either the liquid or the solid phase (whichever the component appears in the design case).

  It is estimated using the formula: $d = a + bT,\ T \text{ in } K.$

  If the mixture is in vapor phase, the system uses the ideal gas law or an equation of state (option available in a few models only) to estimate its density.

- *Purchasing Price* [[$/kg]
  Used in economic calculations. It can be either provided by the user or calculated from the mixture's ingredients as the weighted average of their purchasing price.

# 3.8 Component and Mixture Databanks

As indicated in the beginning of this chapter, Pro-Designer supports up to three different component and mixture databanks. To access the component databanks, use the **Databanks / Pure Components...** menu item from the main menu (or hit **F2** as a shortcut.) In the dialog that comes up (shown in Fig. 3.8), depending on what databank you choose to browse, you will be able to view the properties of a databank component,

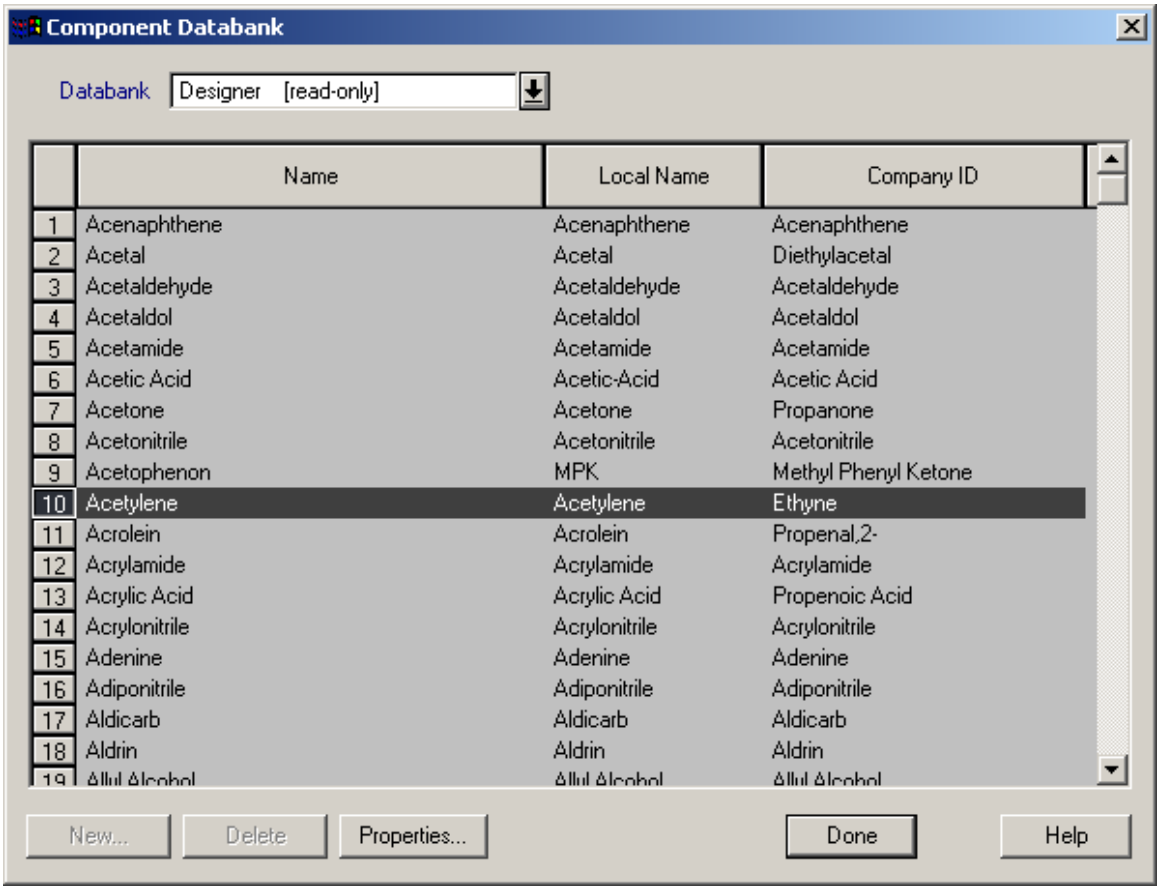


Figure 3.8: The pure component databank dialog.

add a new one, delete or edit an old component. To view or edit a pure component, first select it from the table (by clicking on the button at the beginning of that component's row, i.e. its index column) and then press the **Properties…** button. Alternatively, you can double-click on the component's index column. Note that changes made in the component databanks do not affect existing design cases or other parts of the database unless you attempt to delete a component that is used as a databank stock mixture ingredient. In this case, with the user's consent, the stock mixtures where this component participates as ingredient will be deleted as well.

To access the stock mixture databanks, use the **Databanks / Stock Mixtures...** menu item from the main menu (or hit **Shift + F2** as a shortcut.) The dialog that comes up (shown in Fig. 3.9), depending on what databank you choose to browse, you will be able to view the properties of a databank stock mixture, add a new one, delete or edit an old one. To view or edit a mixture, first select it from the table (by clicking on its index column) and then press the **Properties…** button. Alternatively, you can double-click on the mixture's index column. Note that changes made in the stock mixture databanks do not affect existing design cases or other parts of the database.

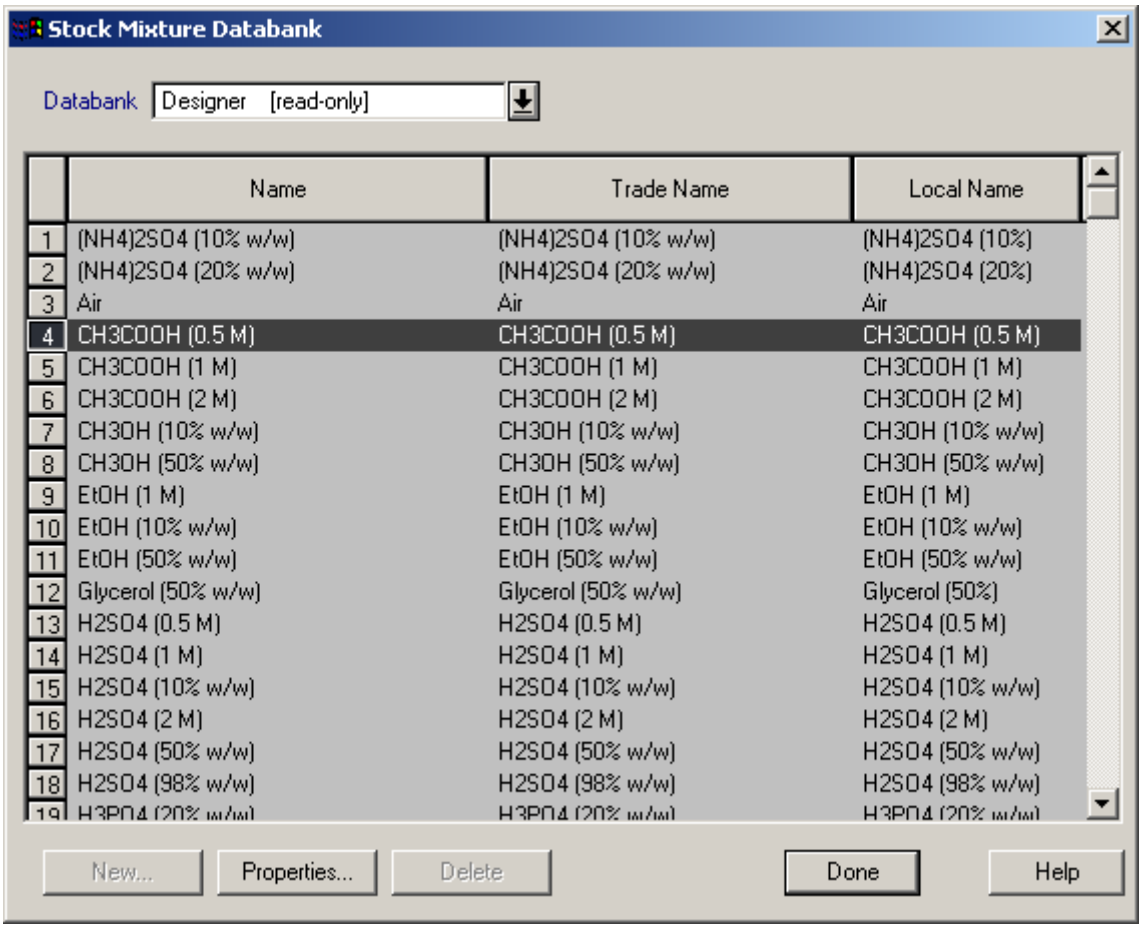


Figure 3.9: The stock mixture databank dialog.

GO TO TOP LEVEL CONTENTS