Part 9

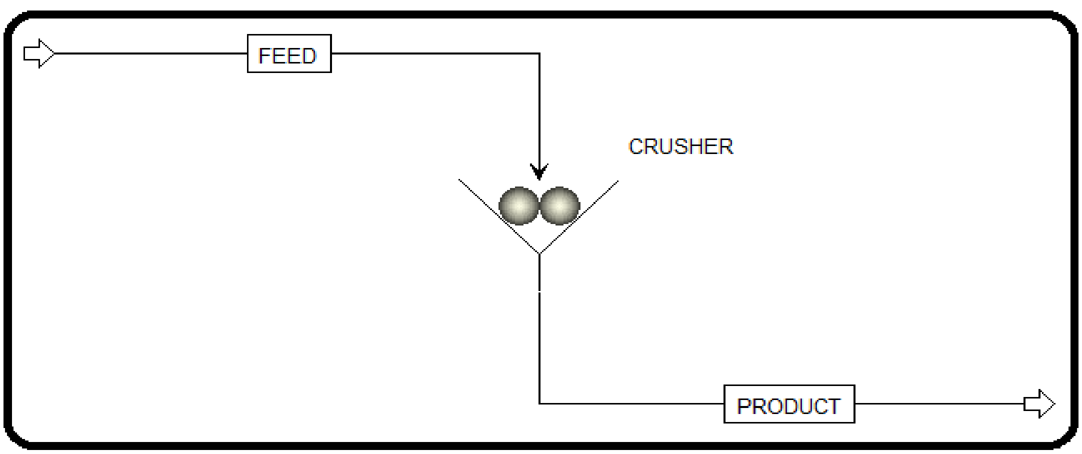
Solid Modelling in Aspen Plus

Problem Definition

Solids handling is important in some chemical industries, such as specialty chemicals (e.g., fertilizers and silicones), extractive processes (e.g., oil shale, copper, and alumina), and biofuel processes (e.g., corn stover and sugarcane).
Unlike liquids, solids handling requires the knowledge of additional characteristics, such as average particle size and density, moisture content, solubility, color, shape, porosity, and particle size distribution, which is usually expressed in terms of the mean particle size and a factor describing the degree of scatter around themean (e.g., standard deviation). Moreover, it is not possible to infer bulk from microscopic (single particles) properties of solids, in general. Aspen Plus has already many useful features that can deal with solids as it perfectly dealt with liquids and gases, as we have seen so far in the previous sessions. Formore information about the different solids unit operations, refer to “APPENDIX”.
Since there are many applications that involve more or less solid materials, we pick up some of them to demonstrate the important features of Aspen Plus in dealing with solidmaterials.

Example: THE CRUSHER

A feed stream of KCL with flowrate of 1250 kg/hr at 20 C and 1 bar with particle size distribution of median 5 mm and standard diviation of 1 mm with upper limit of 10 mm and lower limit of 0 mm passes a crusher which reduces the particle size of the feed stream.

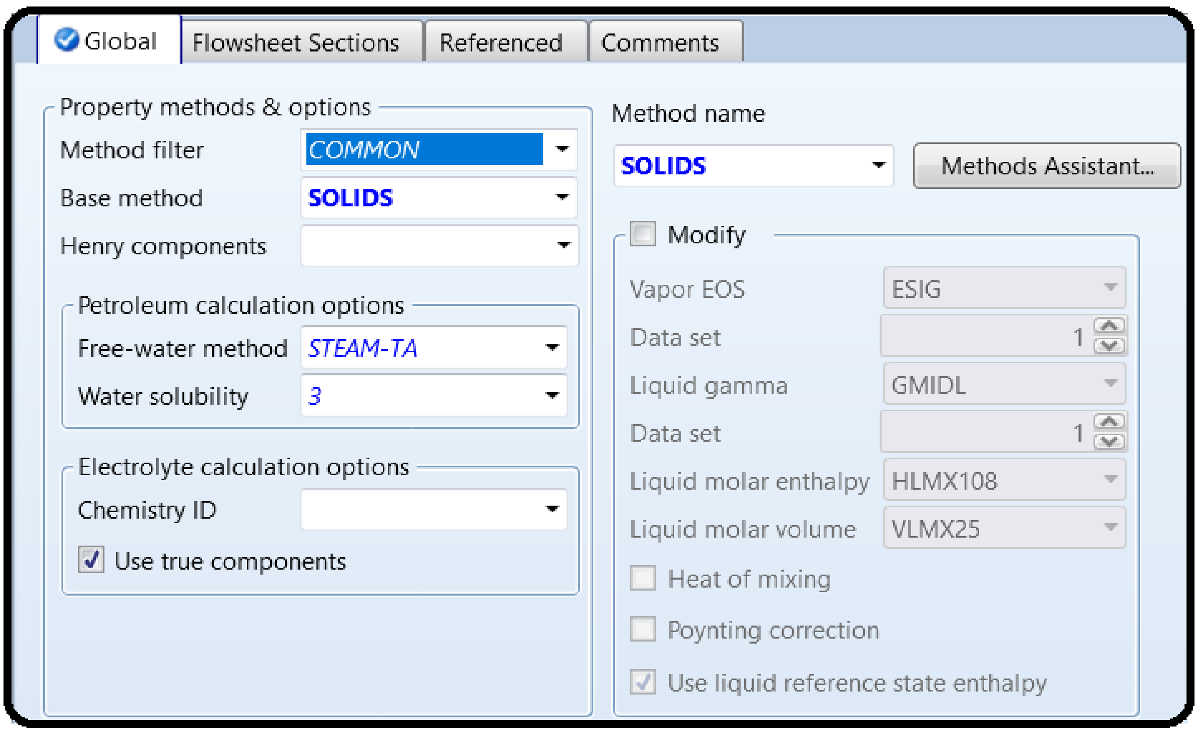


<u>How to simulate</u>

1.Using Aspen Plus, start a new simulation by choosing the “Solids” category and selecting “Solids with Metric Units” template to create a steady-state flowsheet. Notice that Aspen Plus, does not assign a default property method. So, we will set it to “SOLIDS”.

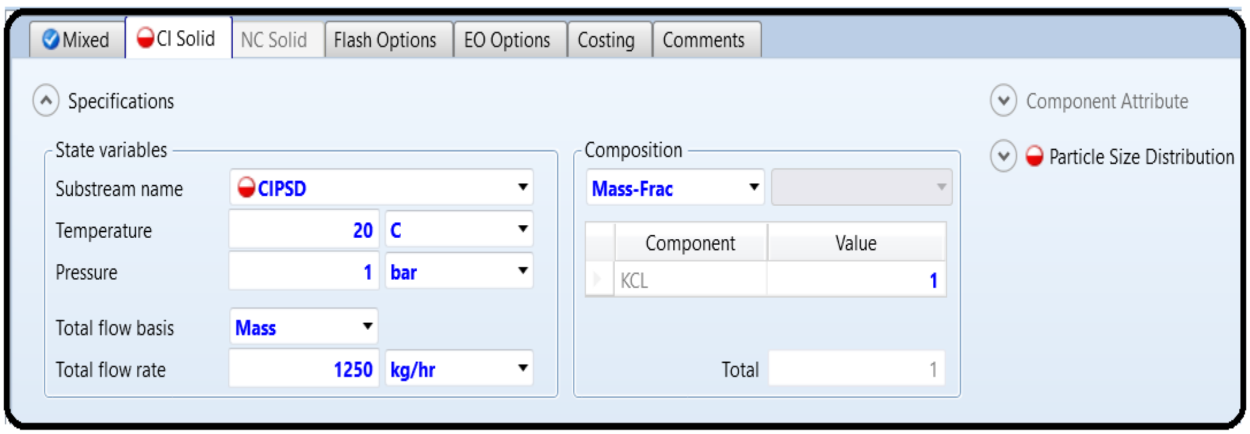
2. In “Navigation” pane menu tree, go to “Components” | “Specifications” | “Selection” sheet. Click on “Find” button to search for “KCL”. Once you find “KCL”, add it to the list of components and change its “Type” from “*Conventional*” to “*Solid*”, as shown in Figure 14.2.

Component ID	Type	Component name	Alias	CAS number
KCL	Solid	POTASSIUM-CHLORIDE	KCL	7447-40-7

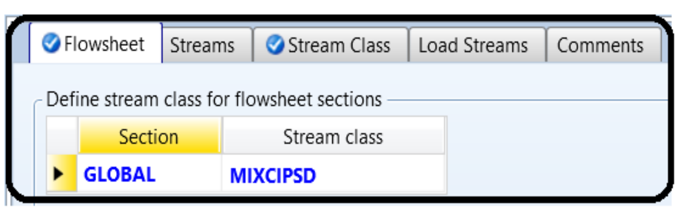


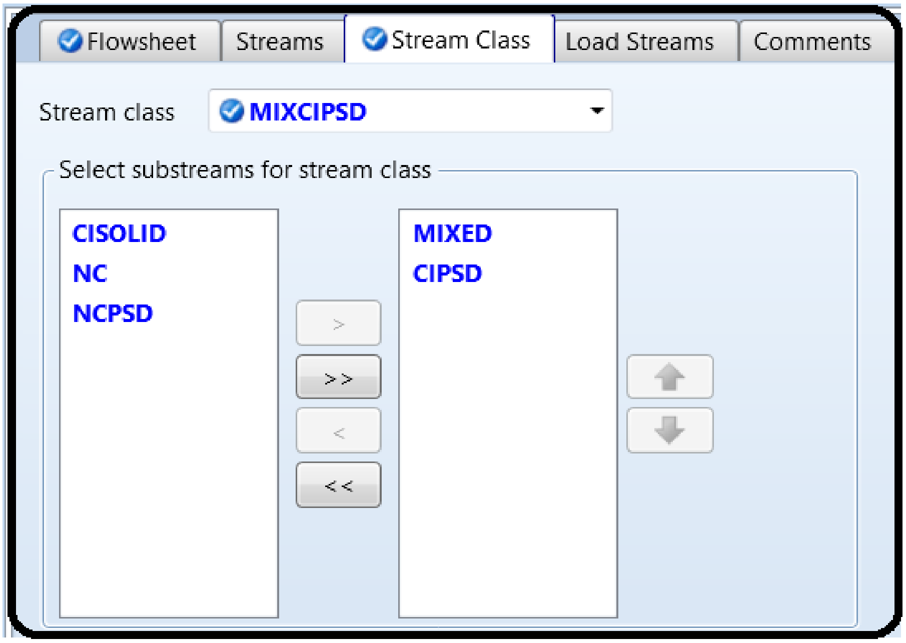
NOTE #1: “KCL” being defined as solid type will be treated as an inert solid with known molecular structure and it will not be involved in aqueous phase equilibrium (i.e., no association/dissociation reactions). However, as we will see shortly that it requires knowledge of further attributes that have to deal with particle size distribution (PSD). Thus, the substream class type for the feed (or product) stream class will be Conventional Inert with PSD (“CIPSD”).

3. Click on “Next” button, run the simulator, and monitor serious warning and errors (if any) via the “Control Panel”. Once you successfully manage to complete the property analysis step, switch to “Simulation” environment.
4. From “Model Palette”, select “Solids” tab, click on “Crusher” icon, and add the crusher icon to the flowsheet area. In addition, add the proper input and output stream, as shown in Figure 14.1. Click on “Next” button and Aspen Plus will bring you to “FEED” stream input form.
Notice here that entering solid-containing feed stream properties are different from those of a conventional feed stream, which has no “Solid” type component. Figure 14.3 shows the typical input data to be entered for a feed stream; however, we will use the second tab, that is, “CI Solid” tab for a conventional inert solid as in our case.



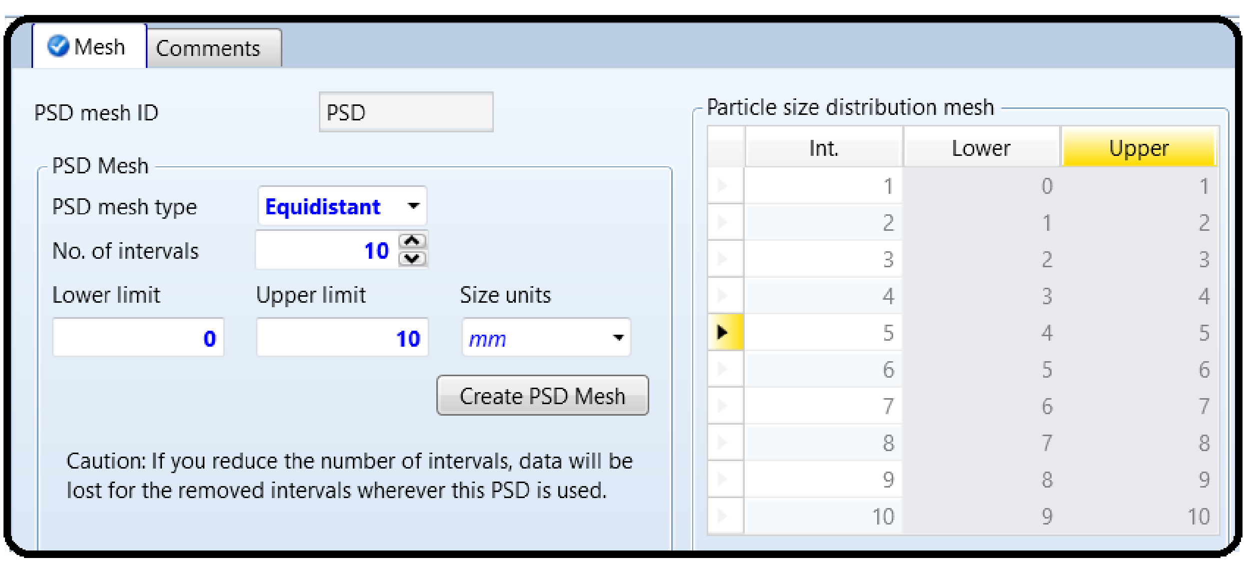
Notice that the half-filled red circle shown in Figure 14.3 indicates that input data pertaining to “FEED” stream is still incomplete, and the reason for this is simply because the stream class is of “MIXCIPSD” type with a substream of “CIPSD” type. Under such stream and substream definitions, we need to define or associate a PSD with the feed stream as well as define a simulation PSD for presentation of results.
5. Figure 14.4 (*top*) shows “Setup” | “Stream Class” | “Flowsheet” tab window where it shows that the stream class for the “Global” section (i.e., entire flowsheet) is of “MIXCIPSD” type. See “APPENDIX” for further information on stream classes. Stream classes ease the integration of solids and fluids in one simulation. The stream class can either be created or selected from a predefined type. Upon one’s need, a predefined class type can also be modified. Moreover, the “Stream Class” tab window (Figure 14.4 *bottom*) shows the selected substream class types for the given stream class of type “MIXCIPSD”. One can select the stream class from the drop-down list and see what substreams are already associated with.





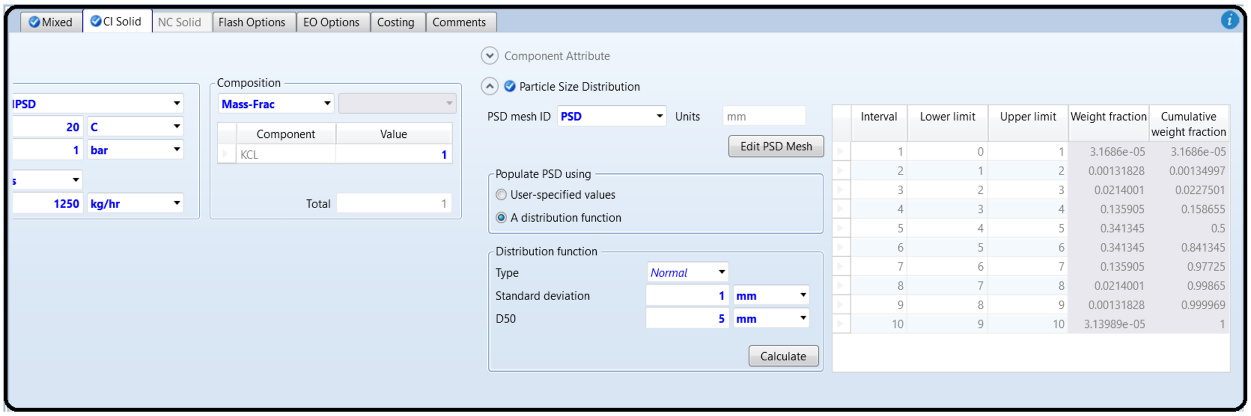
6. Defining the Particle Size Distribution (PSD)

Regarding the particle size distribution (PSD), we will define two PSD types one for the entire simulation and another for the feed stream. Notice here that both PSD types have to be within the same range; that is, the PSD mesh of the simulation within which we monitor the product stream solid attributes should not be too fine or too coarse for the feed stream PSD mesh. So, let us define the simulation PSD first in terms of size unit, lower limit, and upper limit. Figure 14.5 shows that we have selected the "PSD mesh type" to be "*Equidistant*" with parameters as shown in the figure. Do not forget to click on "Create PSD Mesh" button to confirm the creation of the selected PSD.

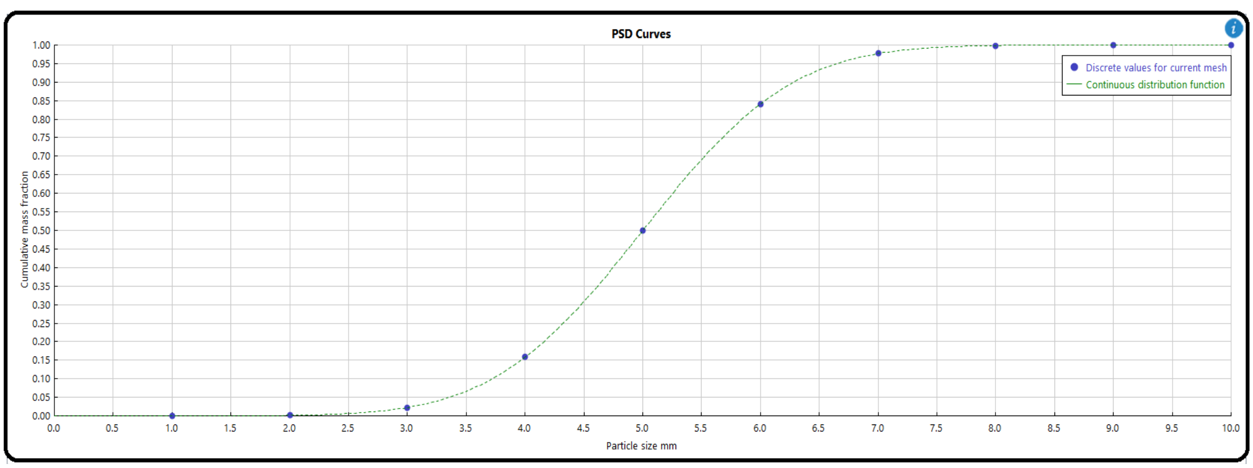


Int.	Lower	Upper
1	0	1
2	1	2
3	2	3
4	3	4
5	4	5
6	5	6
7	6	7
8	7	8
9	8	9
10	9	10

7. Figure 14.6 shows the “CI Solid” tab window for “FEED” stream where we need to define a PSD for the solid of the feed stream. Notice here that you can edit (or modify) the simulation PSD via clicking on “Edit PSD Mesh” button, which will invoke the form shown earlier in Figure 14.5. Moreover, we define a PSD of “FEED” stream, here, as “*Normal*” with a standard deviation of 1mm and median (D50) of 5 mm.

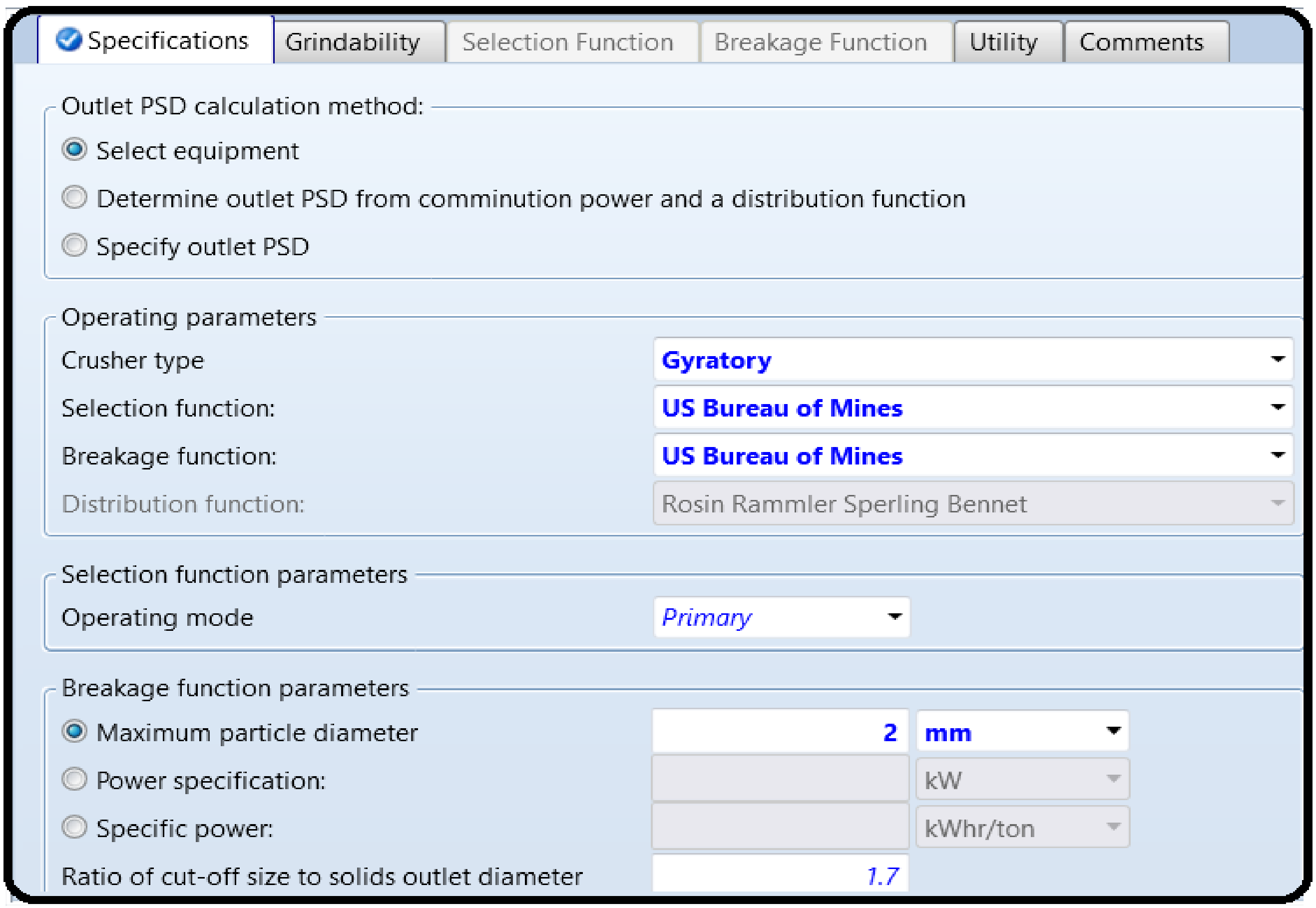


Click on “Calculate” button to generate both the tabulated and graphic representation of PSD for “FEED” stream. Figure 14.7 shows the populated PSD values over the selected PSD mesh, which extends from 0 up to 10mm with equal subintervals. Notice that we have the frequency (i.e., weight fraction) is normally (i.e., symmetrically) distributed around its mean value that lies at about 5 mm. The range of simulation PSD acts like a window through which we have the chance to look at the effect of solids crushing on the PSD of the feed stream.
Figure 14.8 shows the plot of cumulative mass fraction as a function of particle size (mm).

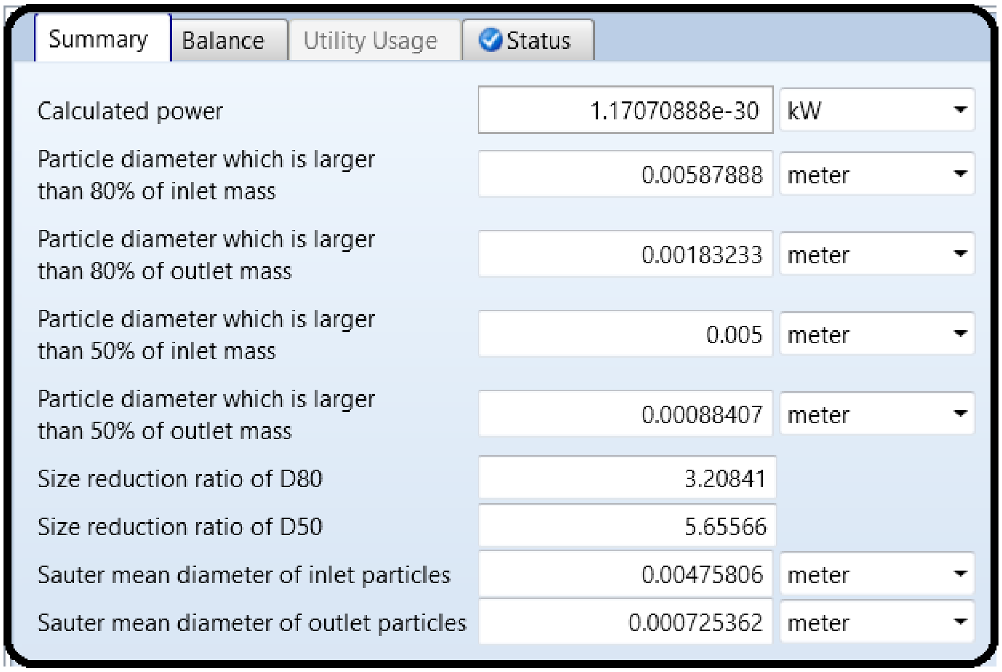


8. Calculation of the Outlet PSD

Click on “Next” button and the “Blocks” | “CRUSHER” | “Input” | “Specifications” tab sheet will show up, as shown in Figure 14.9. The outlet PSD will be calculated based on one of three methods: The first method is to spell out the crusher type, breakage function parameters, impact/rotor velocity, and/or some of its sizing parameters.
The second method is based on known comminution (disintegration) power and some specifie distribution function parameters. Finally, the third method is based on known outlet PSD, which can be either user-specified or common built-in distribution function, such as GGS, RRSB, Normal, and Log normal



9. Click on “Next” button, run the show, and watch out any serious warning or error in“Control Panel”. Figure 14.10 (*left*) shows the “Summary” tab window for “CRUSHER” block under “Results” sheet. Obviously, there is a size reduction between the feed and the outlet stream. The size reduction ratio is 5.656 evaluated at the median. The Sauter mean diameter (see “APPENDIX 14.E”) is also reduced from 4.76 to 0.725 mm. For example, Figure 14.10 (*right*) shows that 98.782% of total particles fall below 3mm diameter size or 99.99997% of them lie below the 4mm diameter dividing cut.



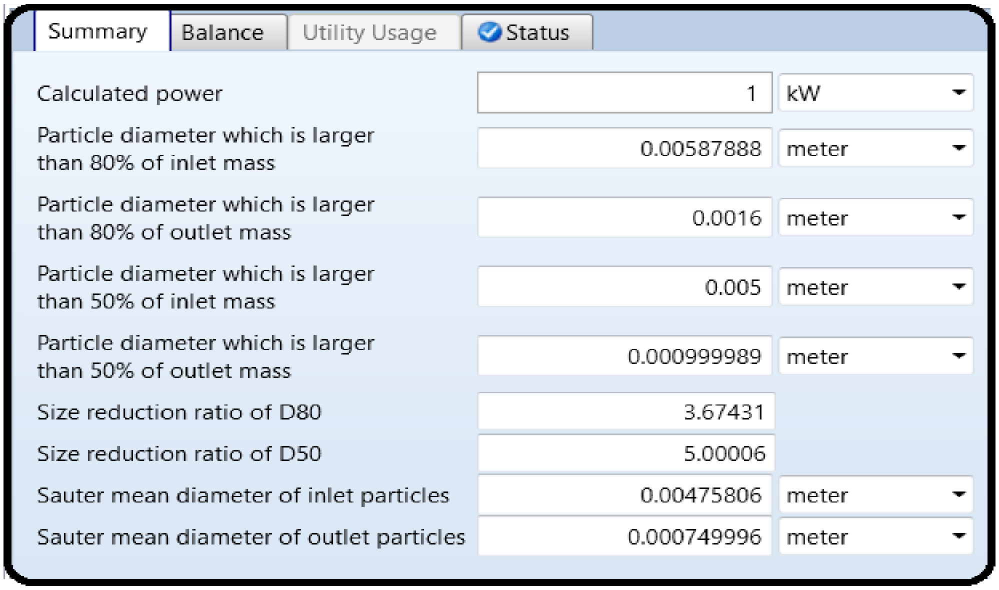
Summary | Balance | Utility Usage | Status

Calculated power	1.17070888e-30	kW
Particle diameter which is larger than 80% of inlet mass	0.00587888	meter
Particle diameter which is larger than 80% of outlet mass	0.00183233	meter
Particle diameter which is larger than 50% of inlet mass	0.005	meter
Particle diameter which is larger than 50% of outlet mass	0.00088407	meter
Size reduction ratio of D80	3.20841	
Size reduction ratio of D50	5.65566	
Sauter mean diameter of inlet particles	0.00475806	meter
Sauter mean diameter of outlet particles	0.000725362	meter

Material | Work | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

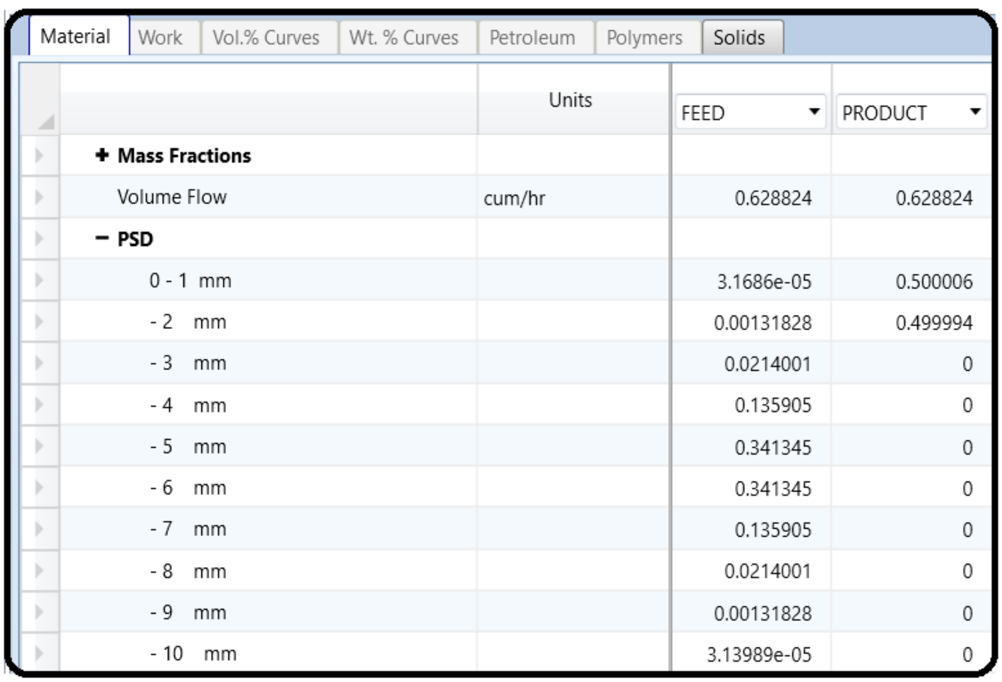
	Units	FEED	PRODUCT
+ Mass Fractions			
Volume Flow	cum/hr	0.628824	0.628824
− PSD			
0 - 1 mm		3.1686e-05	0.565566
- 2 mm		0.00131828	0.281658
- 3 mm		0.0214001	0.140593
- 4 mm		0.135905	0.0121827
- 5 mm		0.341345	0
- 6 mm		0.341345	0
- 7 mm		0.135905	0
- 8 mm		0.0214001	0
- 9 mm		0.00131828	0
- 10 mm		3.13989e-05	0

10. Repeat the same task of reducing the particle size of “FEED” stream but this time using the second method, which is “*Determine outlet PSD from comminution power and a distribution function*” (see Figure 14.9). Under “Specifications” tab, use “*Rosin Rammler Sperling Bennet*” distribution function; power specification of 1kW; and select “*D50*” parameter with “*1mm*” from “Distribution function parameters” option. Under “Grindability” tab, use “*Bond’s law*” as the “Comminution law” and for “CIPSD” substream use “*3 kWhr/ton*” under “Bond work index” column. See Aspen Plus built-in help: “Bond’s Law” for further information on Bond work index. Bond considered that the work necessary for reduction is inversely proportional to the square root of the size produced. This applies for particles between 0.05 and 50 mm.



Summary | Balance | Utility Usage | Status

Calculated power	1	kW
Particle diameter which is larger than 80% of inlet mass	0.00587888	meter
Particle diameter which is larger than 80% of outlet mass	0.0016	meter
Particle diameter which is larger than 50% of inlet mass	0.005	meter
Particle diameter which is larger than 50% of outlet mass	0.000999989	meter
Size reduction ratio of D80	3.67431	
Size reduction ratio of D50	5.00006	
Sauter mean diameter of inlet particles	0.00475806	meter
Sauter mean diameter of outlet particles	0.000749996	meter



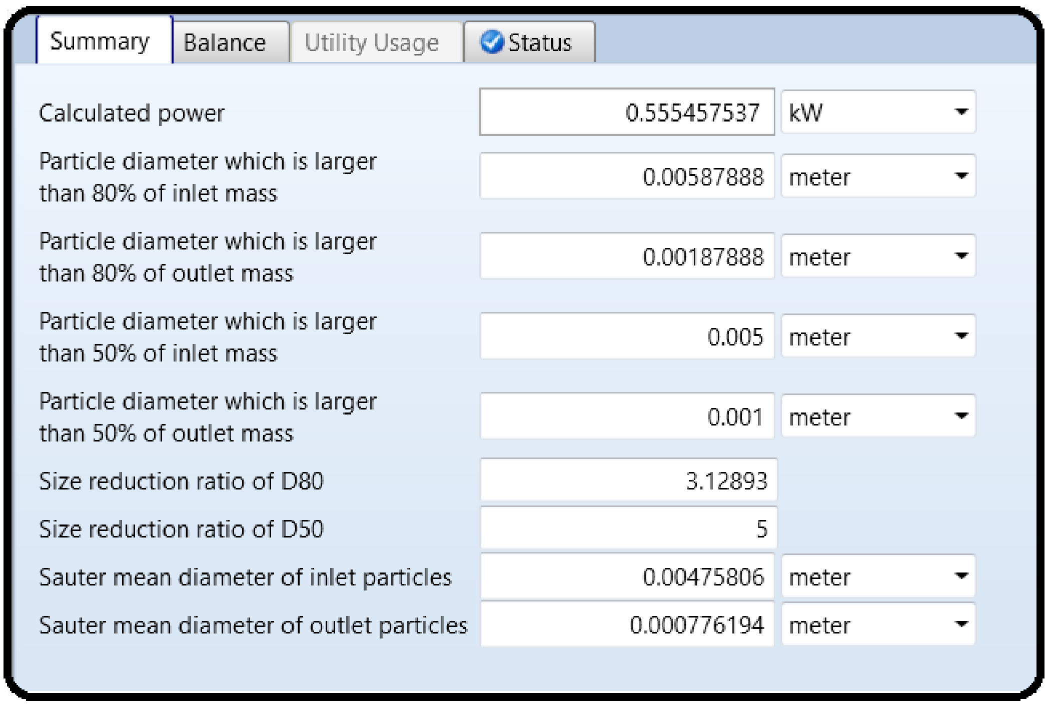
Material | Work | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	FEED	PRODUCT
+ Mass Fractions			
Volume Flow	cum/hr	0.628824	0.628824
− PSD			
0 - 1 mm		3.1686e-05	0.500006
- 2 mm		0.00131828	0.499994
- 3 mm		0.0214001	0
- 4 mm		0.135905	0
- 5 mm		0.341345	0
- 6 mm		0.341345	0
- 7 mm		0.135905	0
- 8 mm		0.0214001	0
- 9 mm		0.00131828	0
- 10 mm		3.13989e-05	0

11. Repeat the same task of reducing the particle size of “FEED” stream but this time using the third method, that is, “*Specify outlet PSD*” (see Figure 14.9). Under “Specifications” tab, select “Substream ID” as *CIPSD*; select “*Use distribution function*”; the “*Bypass fraction*” is set to *0*; create a new distribution function ID and nameit *1*; select the “*Distribution function*” as *Normal*; select D50 parameter with 1mm and standard deviation of 1 mm.
Under “Grindability” tab, you may keep it blank (i.e., no entries at all); however, if you use Bond’s law as the comminution law and for “CIPSD” substream use “*3 kWhr/ton*” under “Bond work index”

column, then you will be able to calculate the power needed to achieve the mission, that is, size reduction of feed stream particles down to the specified outlet PSD.

Report the outlet stream solid attributes in terms of particle size cut, reduction, mean, and distribution (i.e., PSD). Also, report the calculated power (kW) needed to carry out the crushing mission. I hope toward the end of this exercise that you managed to crush the information needed to deal with crushers.



Material / Work / Vol.% Curves / Wt. % Curves / Petroleum / Polymers / Solids	Units	FEED	PRODUCT
+ Mass Fractions			
Volume Flow	cum/hr	0.628824	0.628824
− PSD			
0 - 1 mm		3.1686e-05	0.5
- 2 mm		0.00131828	0.341345
- 3 mm		0.0214001	0.135905
- 4 mm		0.135905	0.0214002
- 5 mm		0.341345	0.00131823
- 6 mm		0.341345	3.13846e-05
- 7 mm		0.135905	2.85665e-07
- 8 mm		0.0214001	9.85308e-10
- 9 mm		0.00131828	1.2792e-12
- 10 mm		3.13989e-05	6.66132e-16

Part 2

Problem Definition

THE FLUIDIZED BED FOR ALUMINADEHYDRATION

In this problem, we will handle the fluidized bed with a chemical reaction. Fluidized beds are used in a variety of industrial processes, which include drying, cooling, heating, and as reactors. The feed stream is made of aluminum trihydroxide (Al(OH)3), which will be dispensed in the form of solid particles to the entrance of the fluidized bed where it will be pneumatically lifted or fluidized by means of a hot air stream. This will cause the phenomenon known as fluidization visualizing solid particles behaving as fluid-like molecules (i.e., they gain the translational, vigorous vibrational, and rotational kinetic energy as well). This being the case, we will enhance the simultaneous mass and heat transfer rates from and to the solid particles. The dehydration reaction

$$2Al\,(OH)3 \rightarrow Al2O3 + 3H2O$$

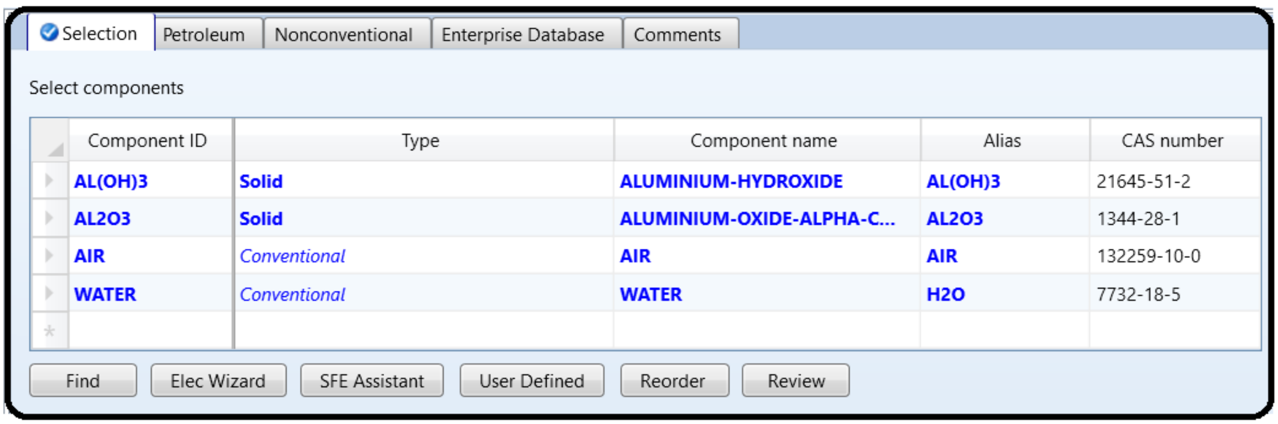
can be put in another form:

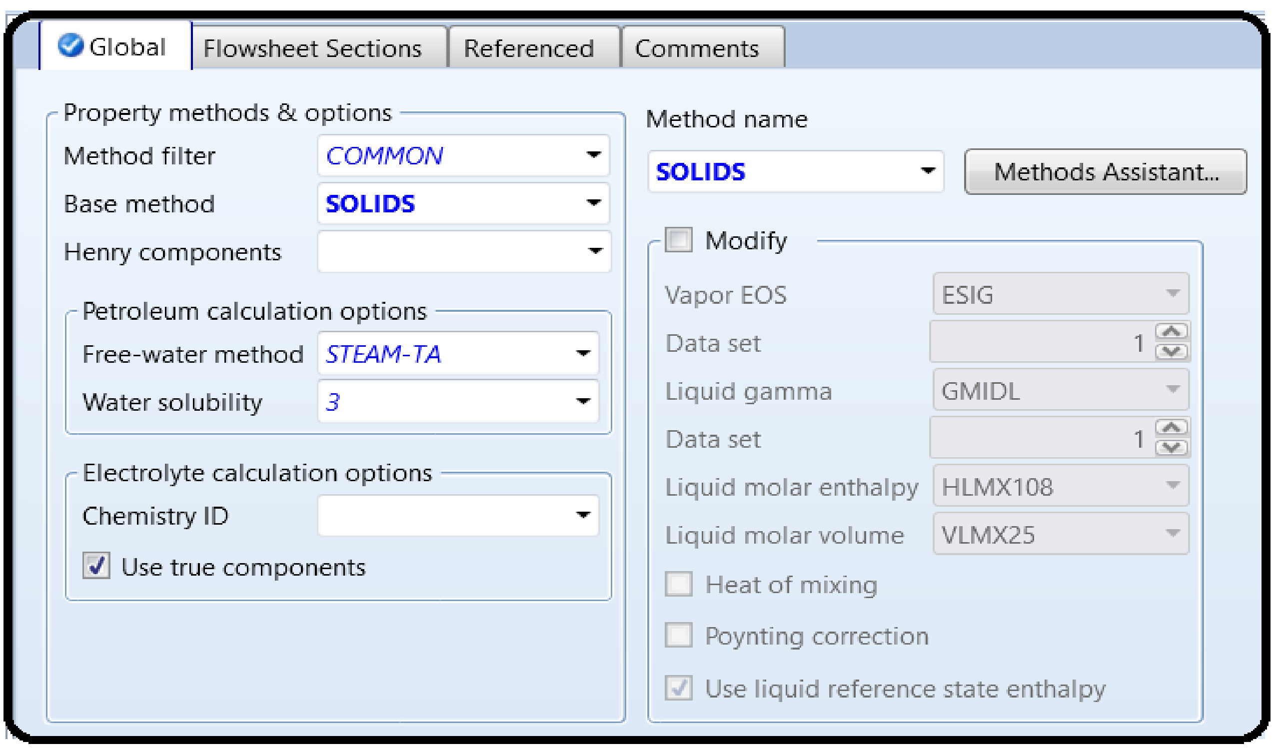
$$Al2O3 \cdot 3H2O \rightarrow Al2O3 + 3H2O$$

So, the reaction is basically a solid transformation from the hydrated into the anhydrous unit crystal. Thus, heating by convection (by the air) and conduction (through the solid particle) will liberate the combined water molecules from the crystal. Keep in mind that this process is a sort of “roasting” process rather than drying. For a typical wet-hydrated alumina or inorganic solids, in general, water molecules are trapped within the solid matrix itself (i.e., within the macropores of a solid pellet, compared with the tiny small size of the unit crystal).

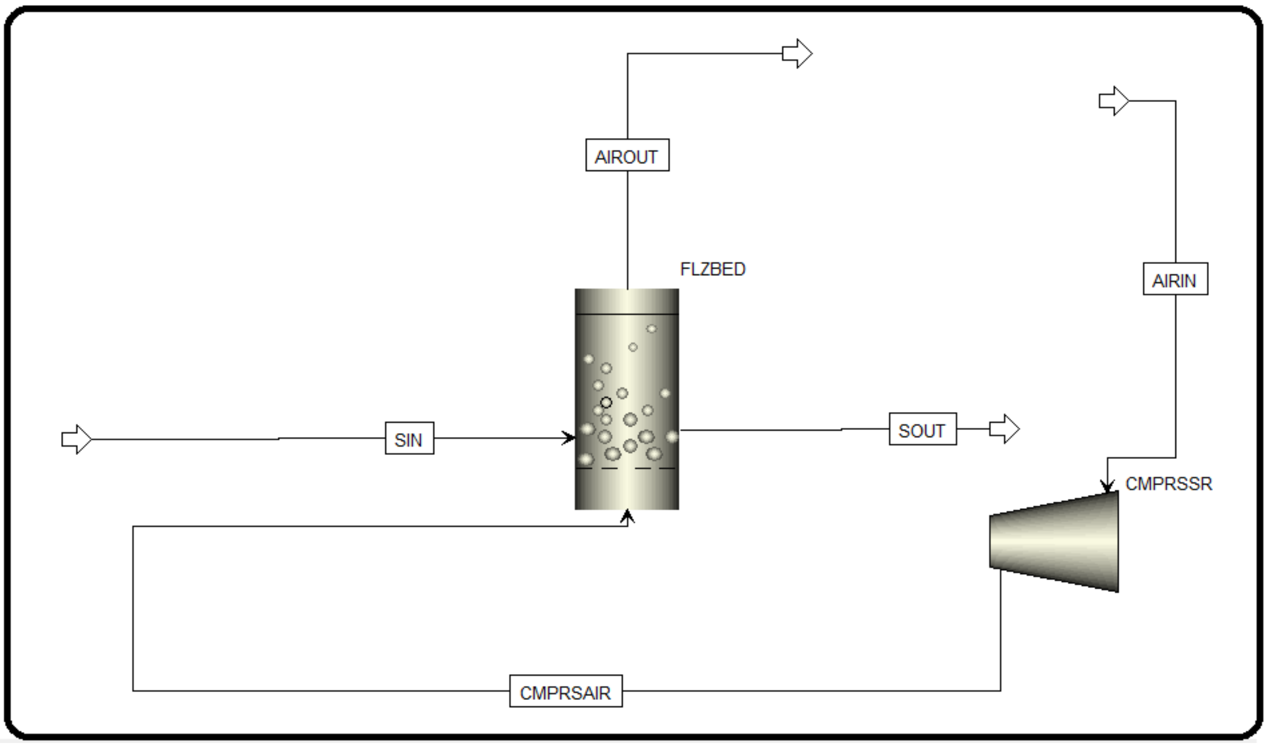
How to Simulate

1. Using Aspen Plus, start a new simulation by choosing the “Solids” category and selecting “Solids with Metric Units” template to create a steady-state flowsheet. We will set the default property method to “SOLIDS”.
2. In “Navigation” pane menu tree, go to “Components” | “Specifications” | “Selection” tab sheet. Add the following components and change the “Type” of both “*AL*(*OH*)*3*” and “*AL2O3*” from “*Conventional*” to “*Solid*”, as shown in Figure 14.11.

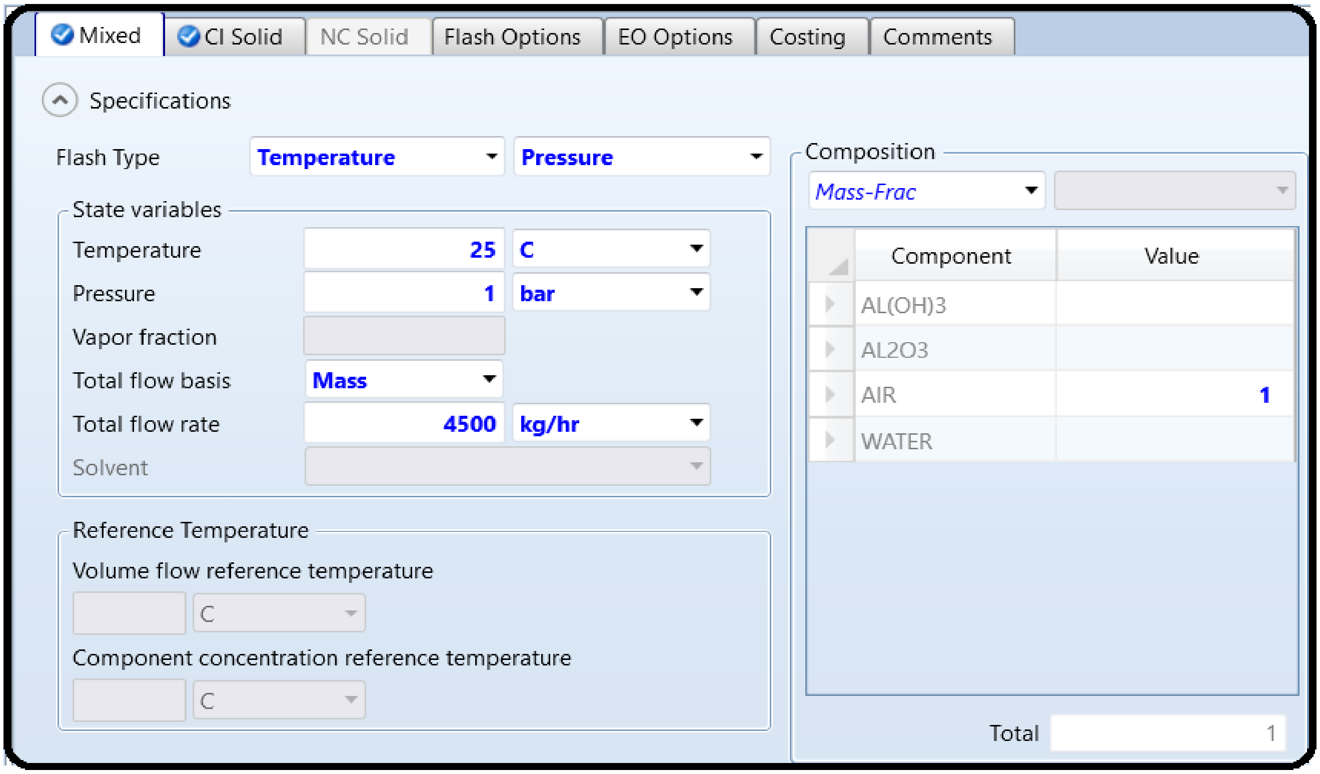


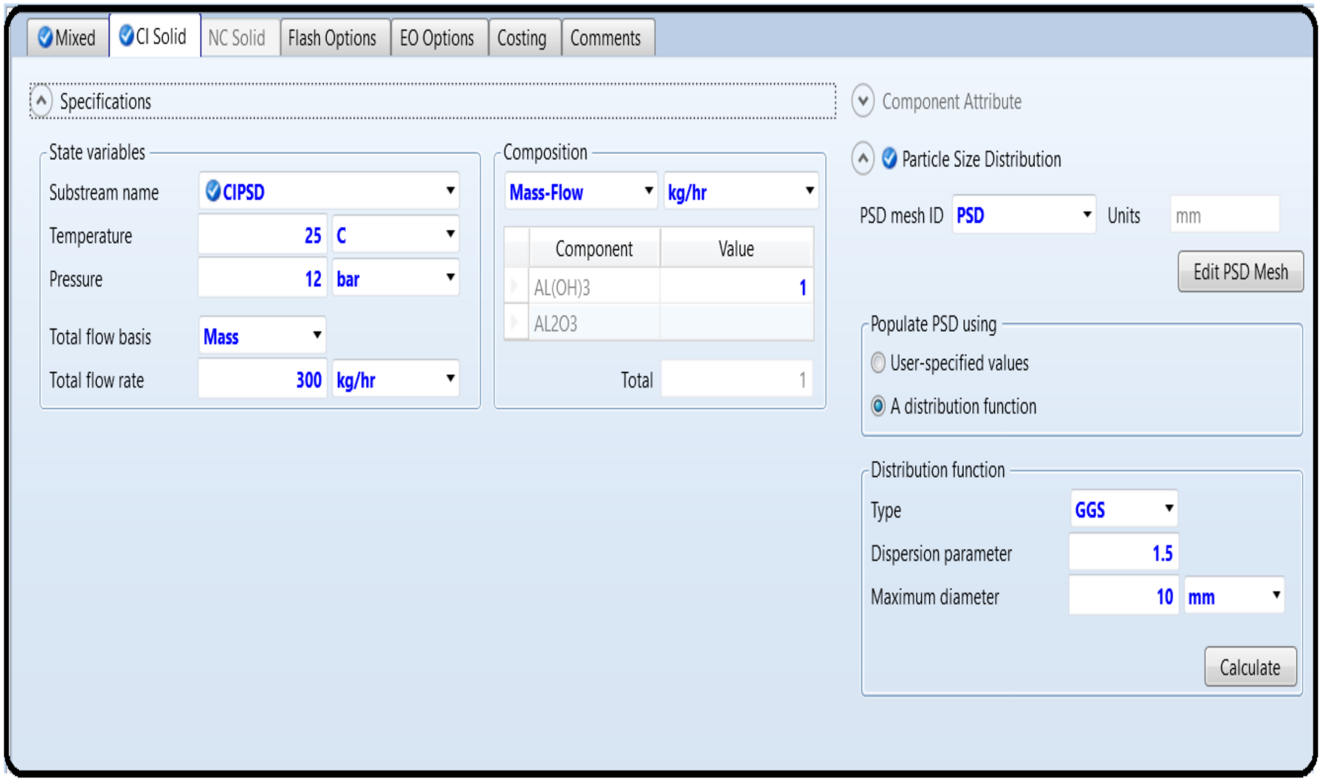


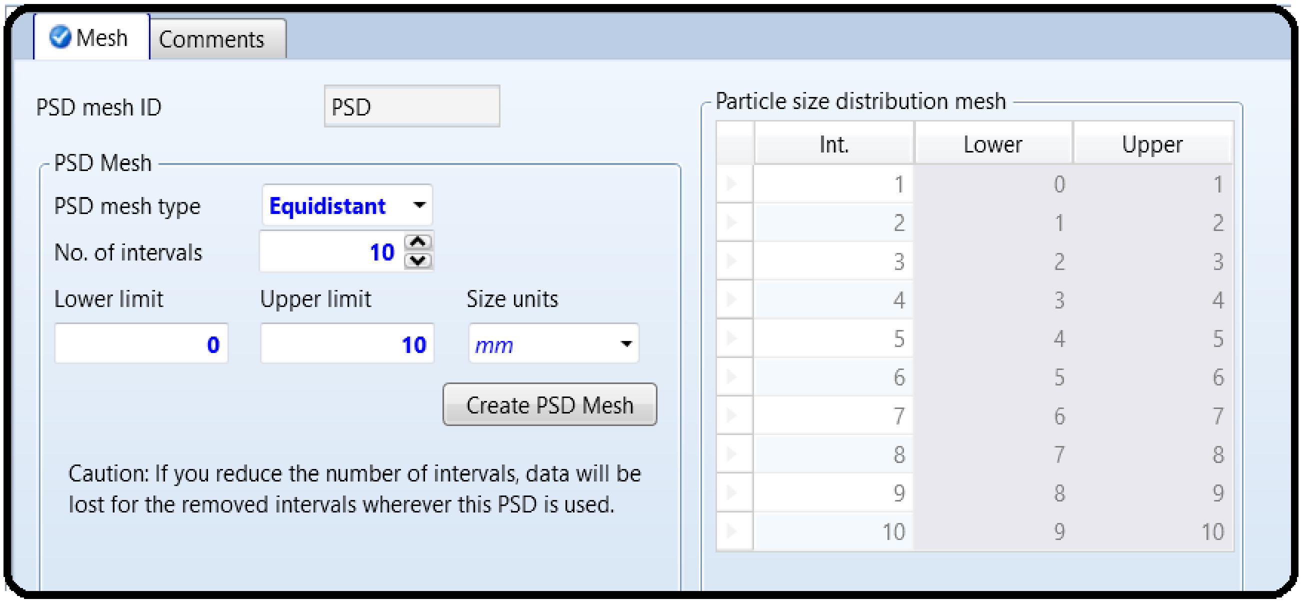
3. Click on “Next” button, run the simulator, and monitor warnings and errors (if any) via the “Control Panel”. Once you successfully manage to complete the property analysis step, switch to “Simulation” environment.
4. From “Model Palette”, select “Solids” tab, click on “Fluidbed” icon, and add the fluidized bed icon to the flowsheet area. Add one compressor unit from “Pressure Changers” tab. In addition, add the proper input and output streams, as shown in Figure 14.12. Notice that “SIN” and “SOUT” stream stand for the inlet and outlet solid streams, respectively.

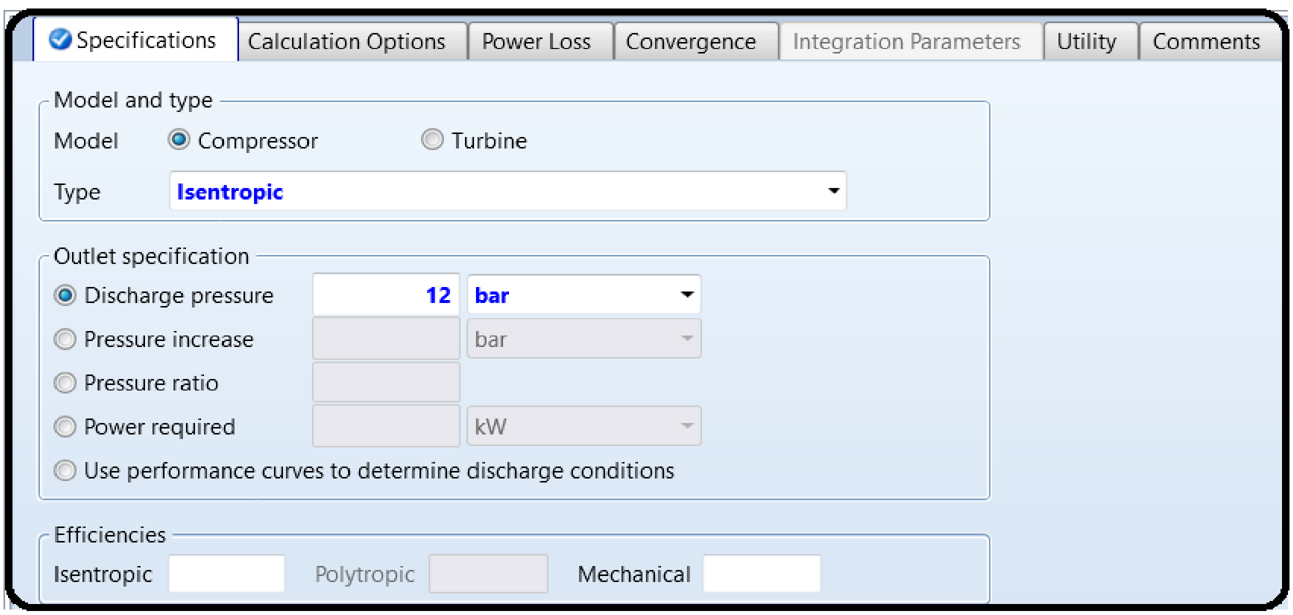


5. Air stream (“**AIRIN**”) will be introduced to the compressor at a rate of 4500 kg/h at room temperature and pressure and the discharge pressure of the compressor will be set at 12 bar. Of course, the temperature of air will increase as a result of adiabatic compression. On the other hand, the solid feed stream (“**SIN**”) will enter at a rate of 300 kg/h at room temperature and a pressure of 12 bar as pure Al(OH)3. Moreover, Figure 14.13 (*left*) shows the simulation PSD mesh and that of “**SIN**” stream (*right*).


Mixed
CI Solid
NC Solid
Flash Options
EO Options
Costing
Comments
Specifications
Flash Type
Temperature
Pressure
State variables
Temperature
25
C
Pressure
1
bar
Vapor fraction
Total flow basis
Mass
Total flow rate
4500
kg/hr
Solvent
Reference Temperature
Volume flow reference temperature
C
Component concentration reference temperature
C
Composition
Mass-Frac
Component
Value
AL(OH)3
AL2O3
AIR
1
WATER
Total
1

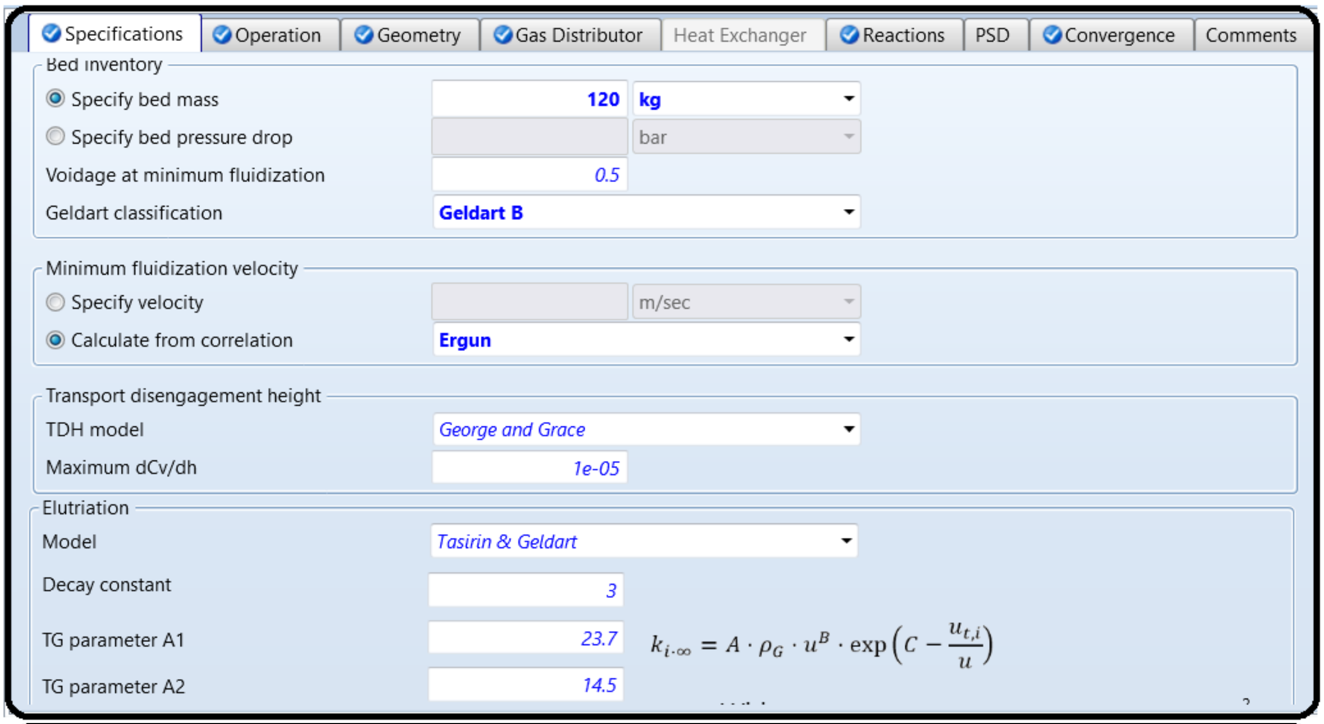

Mixed
CI Solid
NC Solid
Flash Options
EO Options
Costing
Comments
Specifications
State variables
Substream name
CIPSD
Temperature
25
C
Pressure
12
bar
Total flow basis
Mass
Total flow rate
300
kg/hr
Composition
Mass-Flow
kg/hr
Component
Value
AL(OH)3
1
AL2O3
Total
1
Component Attribute
Particle Size Distribution
PSD mesh ID
PSD
Units
mm
Edit PSD Mesh
Populate PSD using
User-specified values
A distribution function
Distribution function
Type
GGS
Dispersion parameter
1.5
Maximum diameter
10
mm
Calculate

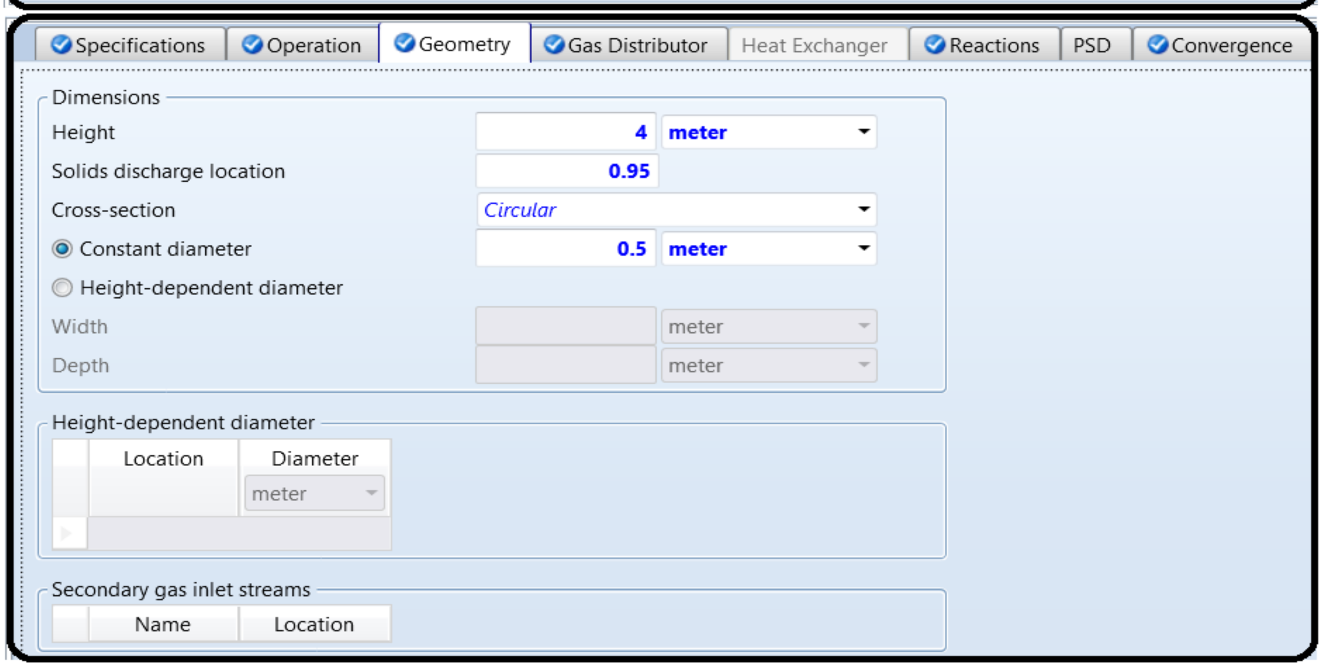


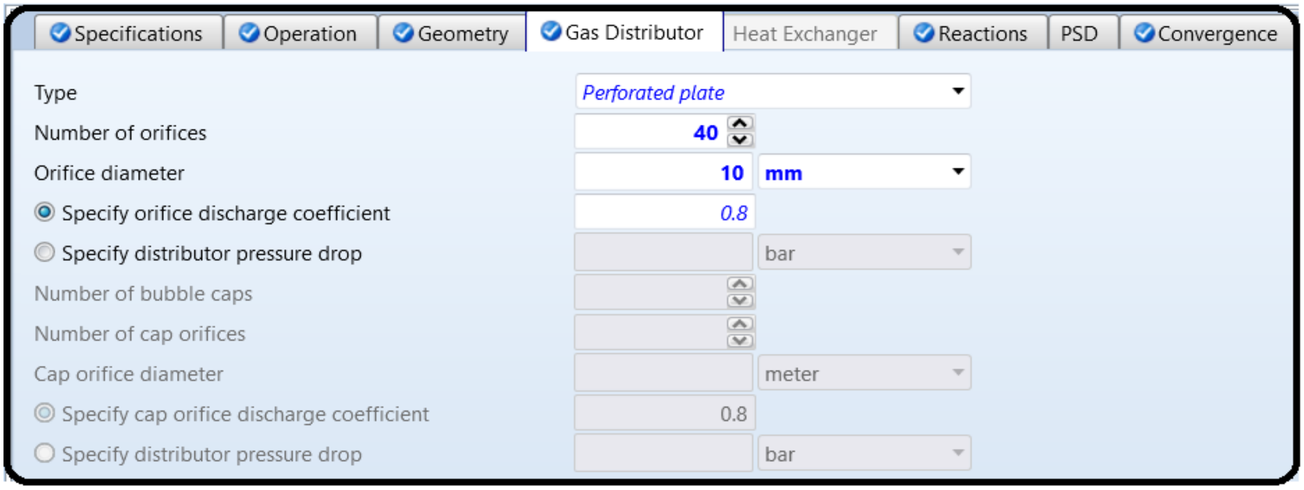


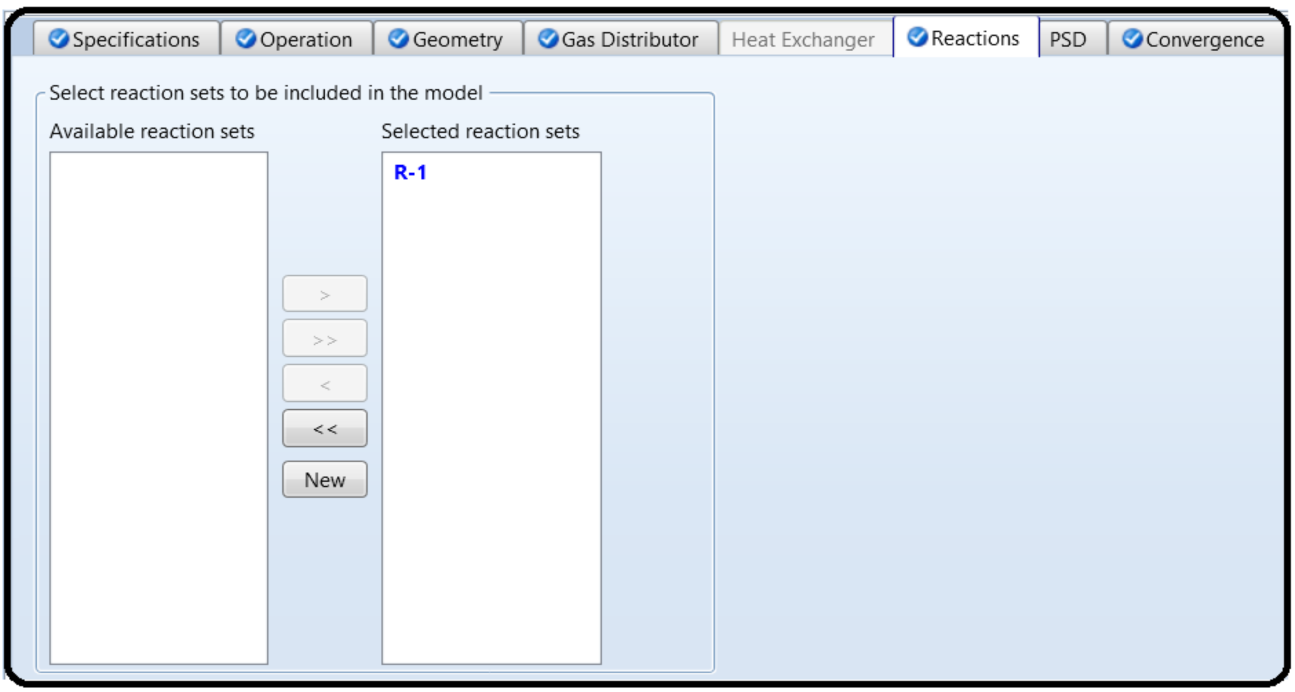
6.For the fluidized bed block, the following design specifications are entered, as shown in Figure 14.14. First, under "Specifications" tab, the bed mass is set to *120 kg*; "*Geldart B*" classification; and "*Ergun*" model for finding the minimum fluidization velocity. Second, under "Geometry" tab, the bed height is set to *4m*; the solid discharge location *0.95* (i.e.,0.95 × 4=3.8m, measured from the bottom of the bed); and the cross-sectional area with a constant diameter equal to *0.5m*. Third, under "Gas Distributor" tab, its type is set to "*Perforated plate*" with number of orifices equal to *40*, diameter equal to *10*mm each, and the default orifice discharge coefficient of *0.8*. Fourth, under "Convergence" tab, for mass balance convergence, the solver is set to "*Newton*" instead of

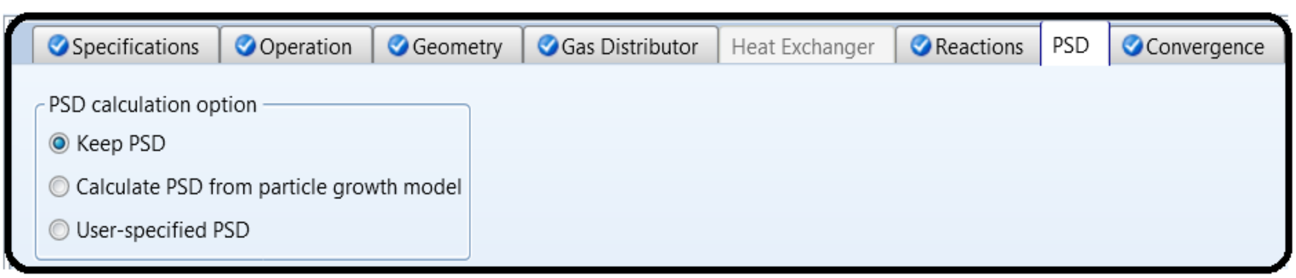
"*Broyden*", as the latter did not properly converge for a reasonable solution for the given fluidization case. Finally, under "Reactions" tab we will associate the reaction "R-1" set to the fluidized bed. The reaction "R-1" set will be created shortly.

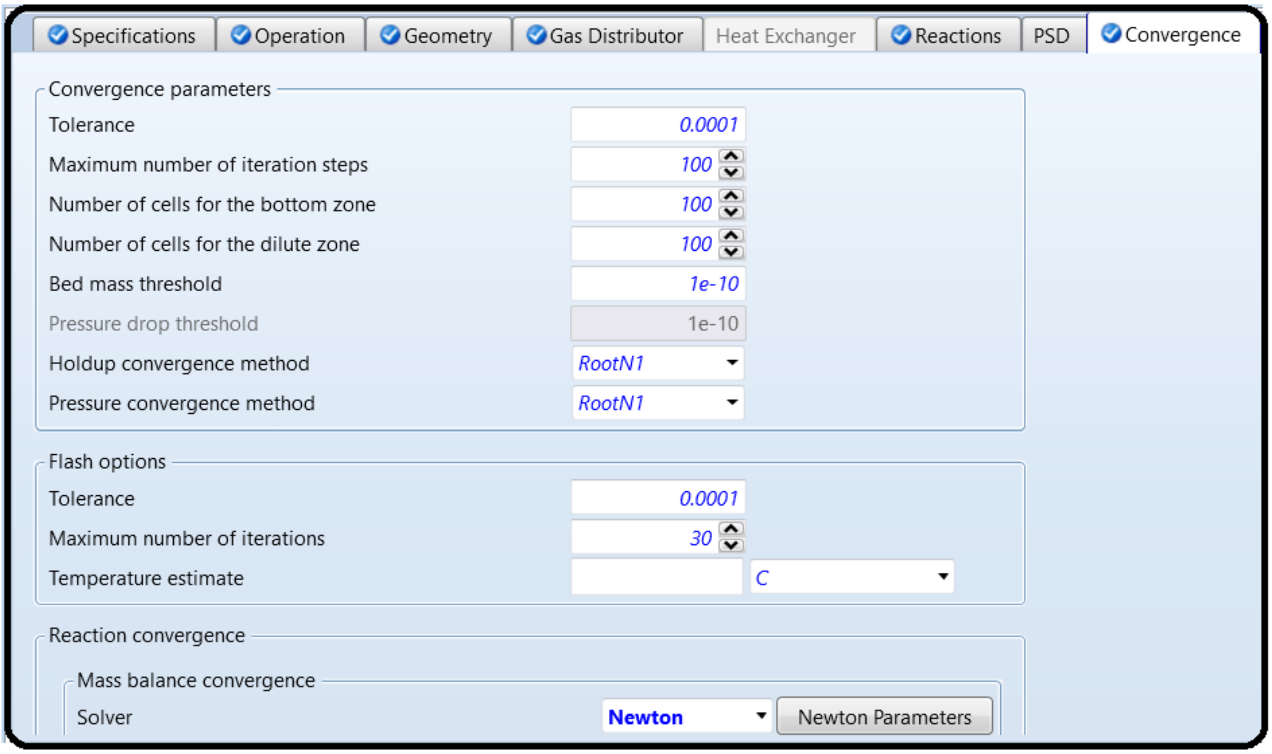




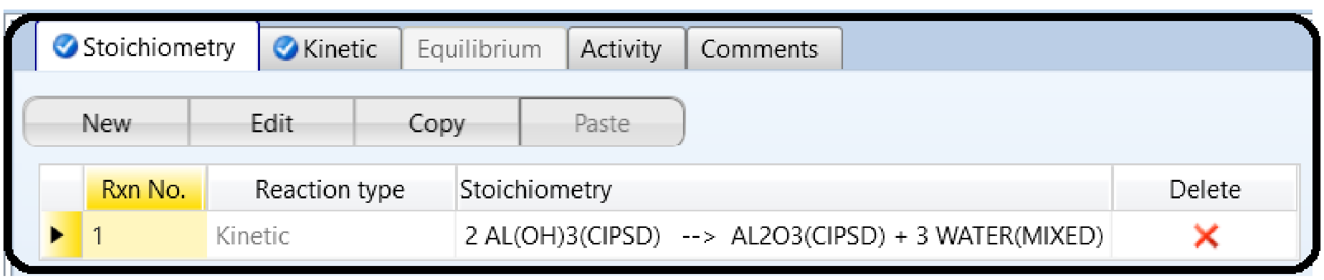

Specifications
Operation
Geometry
Gas Distributor
Heat Exchanger
Reactions
PSD
Convergence
Type
Perforated plate
Number of orifices
40
Orifice diameter
10
mm
Specify orifice discharge coefficient
0.8
Specify distributor pressure drop
bar
Number of bubble caps
Number of cap orifices
Cap orifice diameter
meter
Specify cap orifice discharge coefficient
0.8
Specify distributor pressure drop
bar

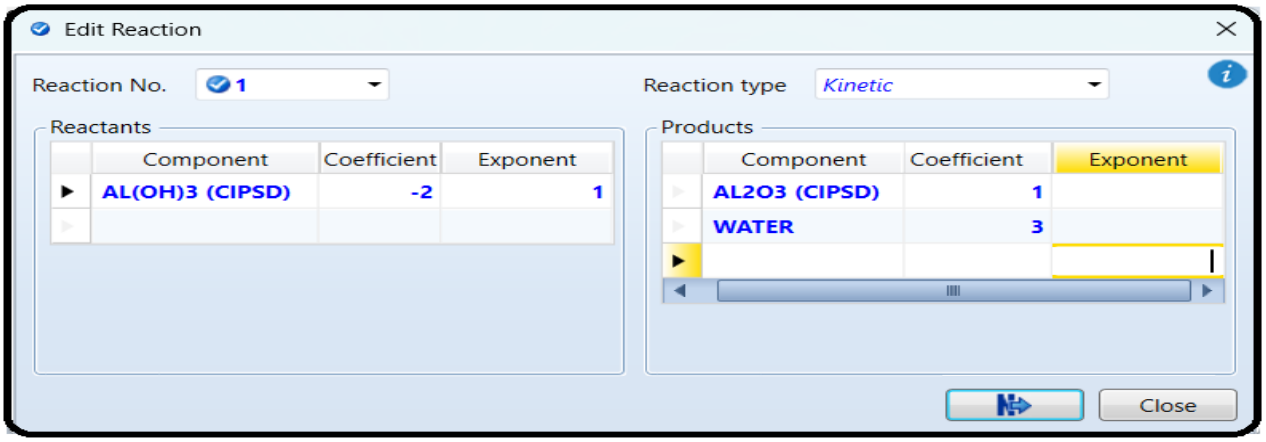

Specifications
Operation
Geometry
Gas Distributor
Heat Exchanger
Reactions
PSD
Convergence
Select reaction sets to be included in the model
Available reaction sets
Selected reaction sets
R-1
>
>>
<
<<
New

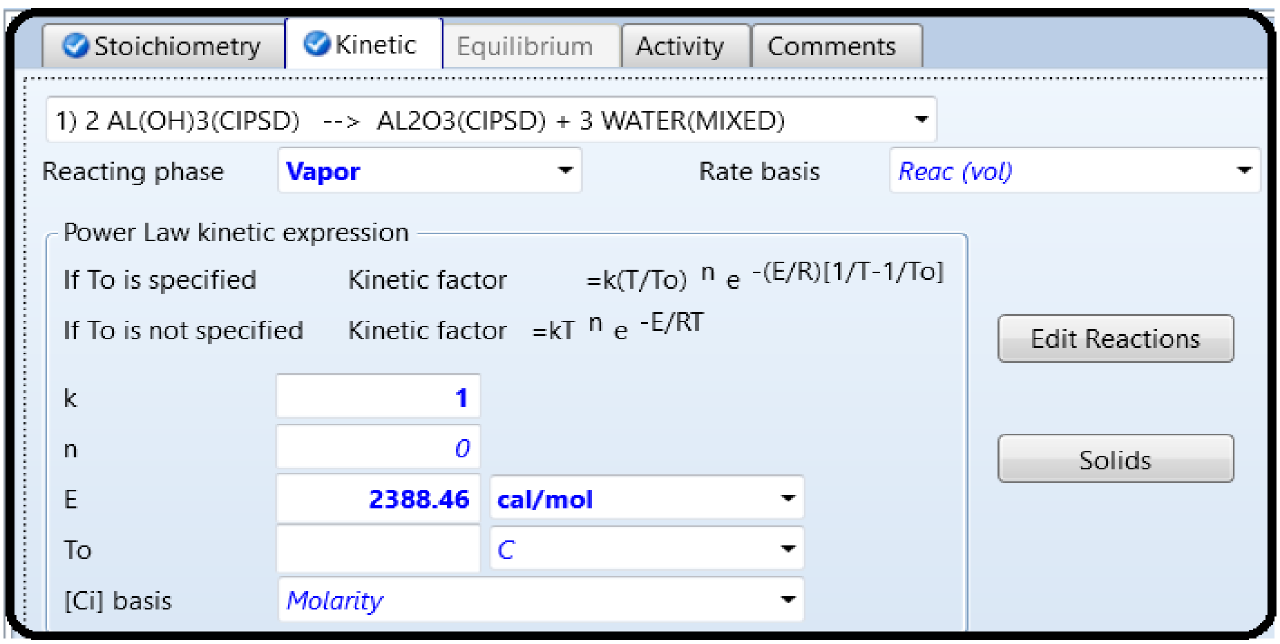

Specifications
Operation
Geometry
Gas Distributor
Heat Exchanger
Reactions
PSD
Convergence
PSD calculation option
Keep PSD
Calculate PSD from particle growth model
User-specified PSD



The reaction "**R-1**" set will be created under "**Reactions**" folder. Figure 14.15 shows the stoichiometry and kinetic data associated with alumina transformation from a hydrous to anhydrous state.




Edit Reaction
Reaction No.
1
Reaction type
Kinetic
Reactants
Component
Coefficient
Exponent
AL(OH)3 (CIPSD)
-2
1
Products
Component
Coefficient
Exponent
AL2O3 (CIPSD)
1
WATER
3
Close


Stoichiometry
Kinetic
Equilibrium
Activity
Comments
1) 2 AL(OH)3(CIPSD) --> AL2O3(CIPSD) + 3 WATER(MIXED)
Reacting phase
Vapor
Rate basis
Reac (vol)
Power Law kinetic expression
If To is specified
Kinetic factor
=k(T/To) n e -(E/R)[1/T-1/To]
If To is not specified
Kinetic factor
=kT n e -E/RT
k
1
n
0
E
2388.46
cal/mol
To
C
[Ci] basis
Molarity
Edit Reactions
Solids

<u>Results</u>

Figure 14.16 (*left*) shows the results summary of the calculated geometrical and operational variables of the fluidized bed and the moisture profile of air stream where dry air enters at the bottom and becomes moist as it moves upward (*right*).

Summary | Balance | Profiles | Gas compositions | Status

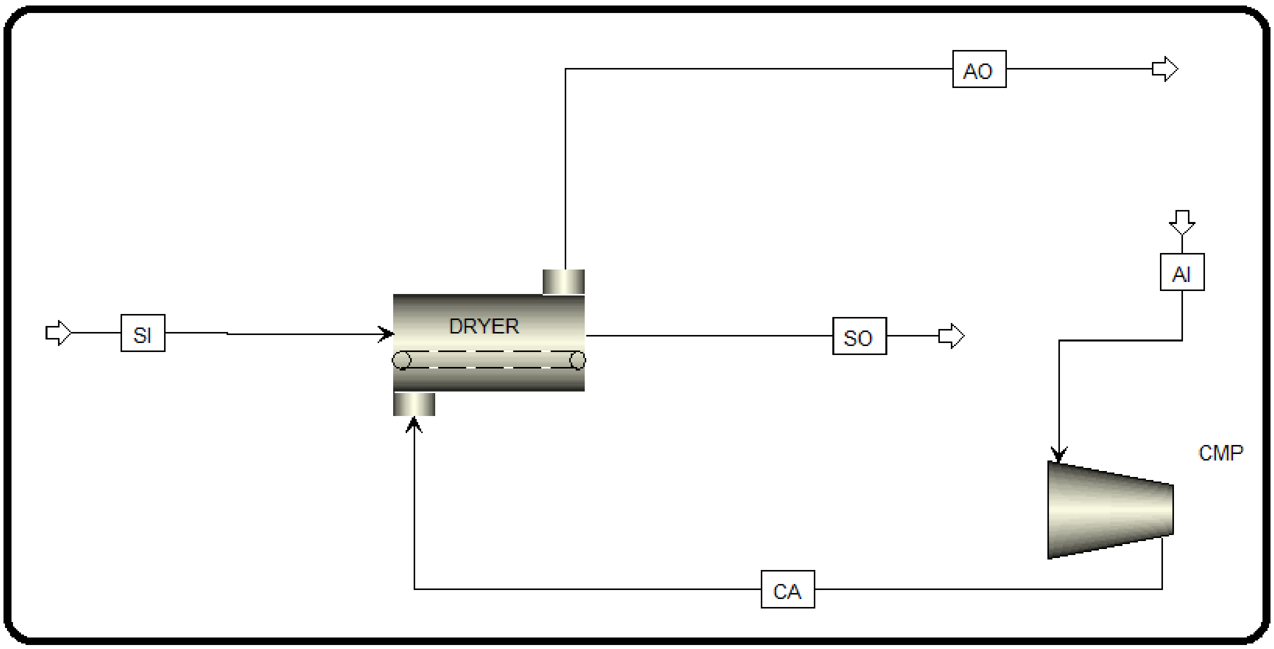
Height of bottom zone	0.108436	meter
Height of freeboard	3.89156	meter
TDH calculated from correlation	2.19969	meter
TDH based on solids volume fraction profile	3.85265	meter
Solids holdup	119.998	kg
Number of particles in bed	1.60882e+07	
Surface area	48.3044	sqm
Distributor pressure drop	0.211705	bar
Bottom zone pressure drop	0.0154238	bar
Freeboard pressure drop	0.0469366	bar
Fluidized bed pressure drop	0.0623604	bar
Overall pressure drop	0.274065	bar
Heat duty	0	Gcal/hr
Minimum fluidization velocity	0.704601	m/sec
Calculated temperature	353.468	C
Moles generated	3.84505	kmol/hr

Material	Units	CMPRSAIR	SIN	AIROUT	SOUT
Total Stream					
Temperature	C	442.065	25	353.468	353.468
Pressure	bar	12	12	11.7259	11.7261
Molar Vapor Fraction		1	0	0.999999	0
Molar Liquid Fraction		0	0	0	0
Molar Solid Fraction		0	1	5.92826e-07	1
Mass Vapor Fraction		1	0	0.999998	0
Mass Liquid Fraction		0	0	0	0
Mass Solid Fraction		0	1	2.11621e-06	1
Molar Enthalpy	kcal/mol	2.97075	-304.767	0.267563	-391.763
Mass Enthalpy	kcal/kg	102.614	-3907.1	9.36854	-3842.71
Molar Entropy	cal/mol-K	1.292	-96.9643	0.325636	-56.6278
Mass Entropy	cal/gm-K	0.0446271	-1.24308	0.0114019	-0.555448
Molar Density	mol/cc	0.000201798	0.031024	0.00022507	0.0390551

Part 3

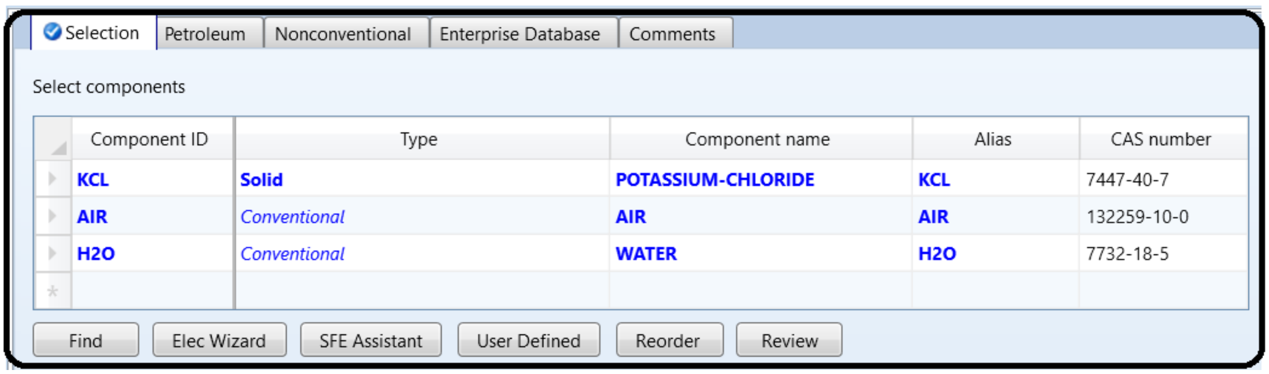
Problem Definition: KCL DRYING

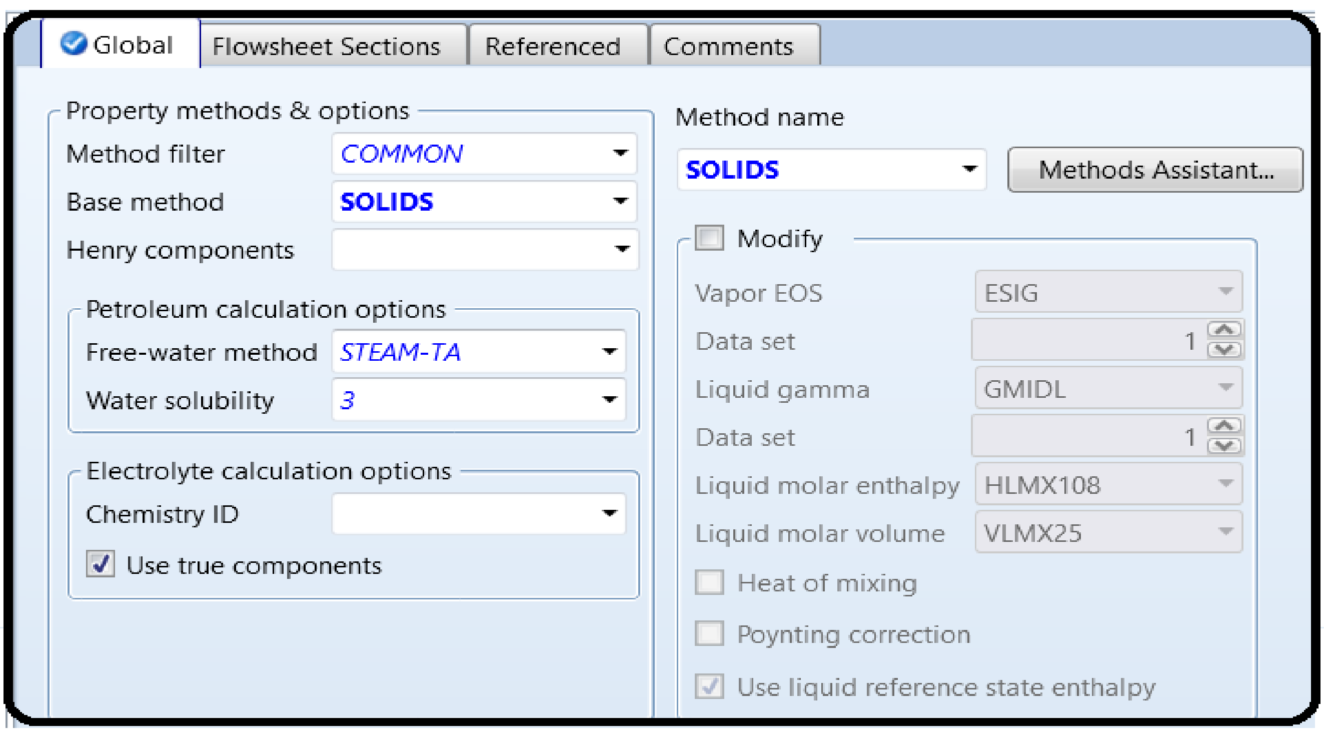
Consider the process of KCl drying using hot air, where moisture will migrate from the wet solid to the dry air and the heat needed will be convectively supplied by the hot air.



How to Simulate

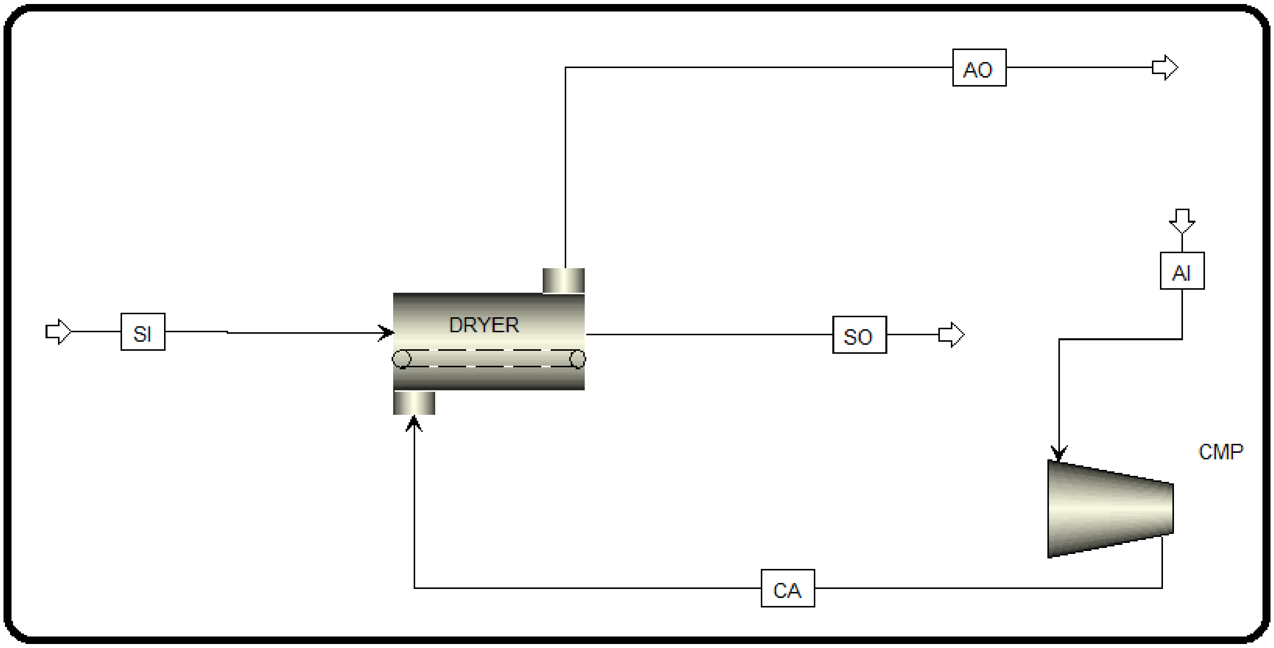
1. Using Aspen Plus, start a new simulation by choosing the “Solids” category and selecting “Solids with Metric Units” template to create a steady-state flow sheet. Notice that Aspen Plus does not assign a default property method. So, we will set it to “SOLIDS”.
2. In “Navigation” pane menu tree, go to “Components” | “Specifications” | “Selection” sheet. Click on “Find” button to search for “KCL”. Once you find “KCL”, add it to the list of components and change its “Type” from “*Conventional*” to “*Solid*”. Add water and air as well, as shown in Figure 14.18.





3. Click on “Next” button, run the simulator, and monitor warnings and errors (if any) via the “Control Panel”. Once you successfully manage to complete the property analysis step, switch to “Simulation” environment. From “Model Palette”, select “Solids” tab, click on “Dryer” icon, and add

the dryer icon to the flowsheet area. Add one compressor unit from “Pressure Changers” tab. In addition, add the proper input and output streams, as shown in Figure 14.19.



Under “**Solids**” folder, selectwater as the moisture component, as shown in Figure 14.20.

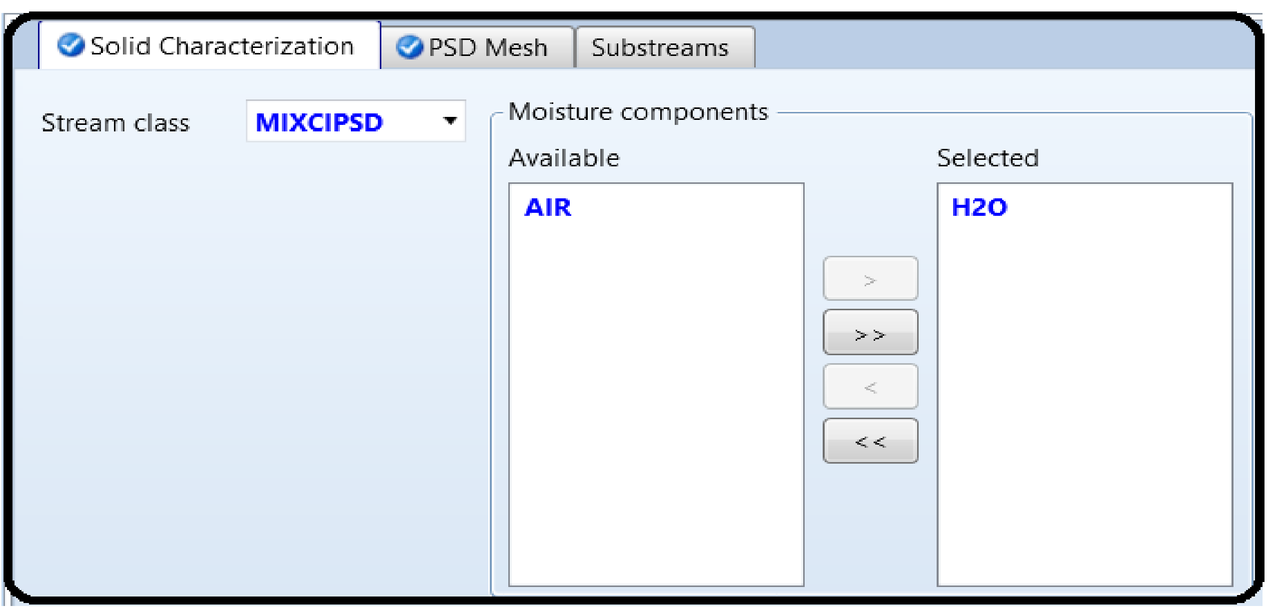


Figure 14.21 shows the creation of a simulation PSD mesh for monitoring the effect of drying on the particle size distribution of the substance being dried.

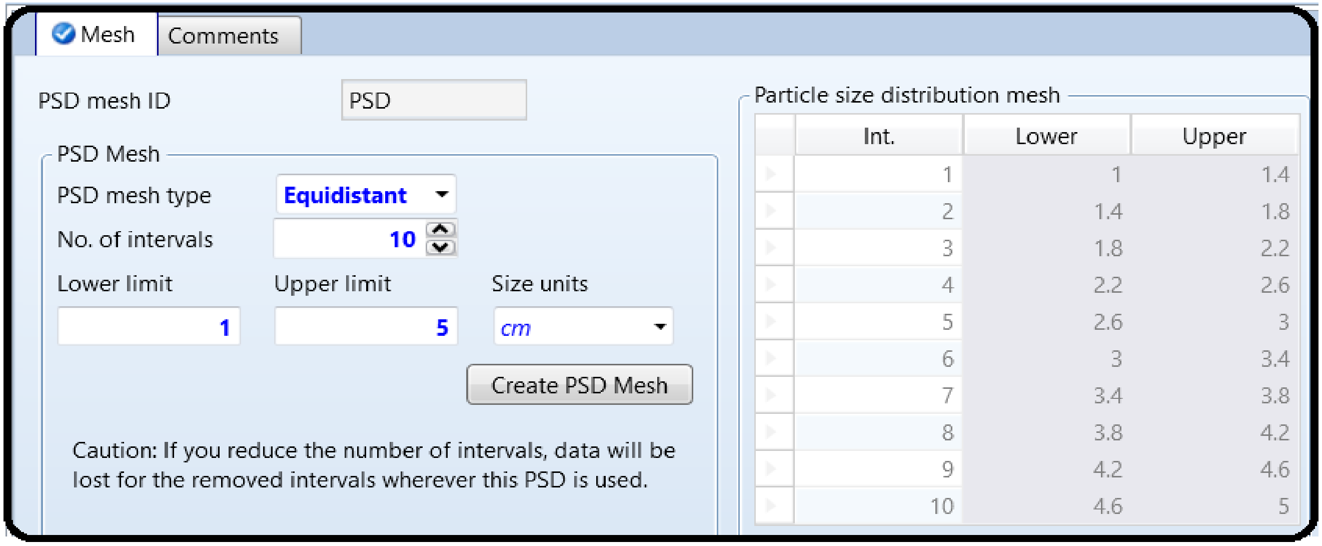
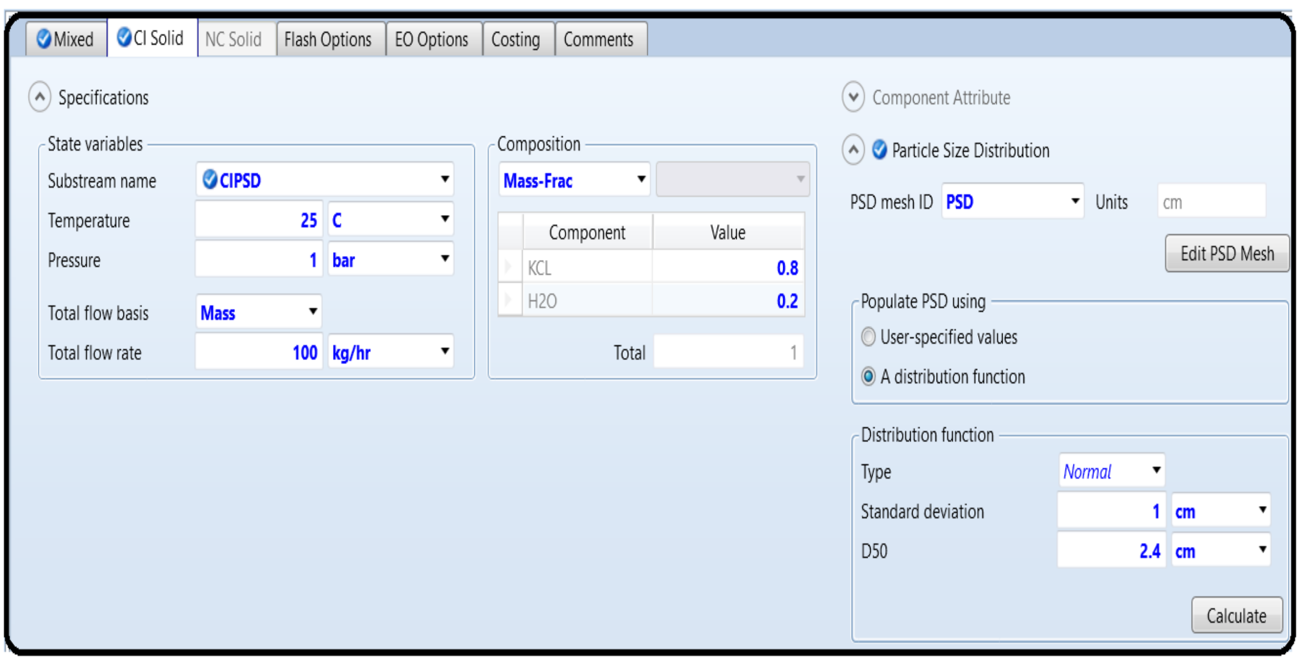
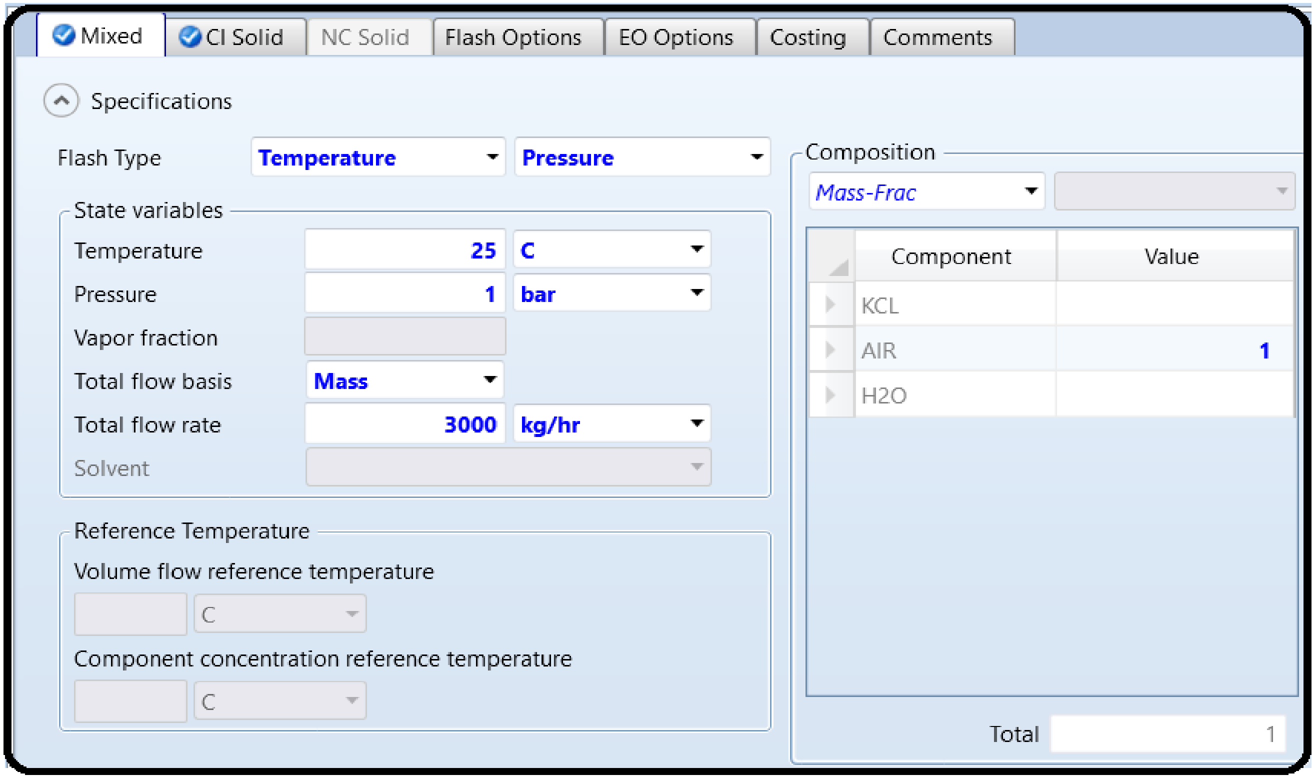


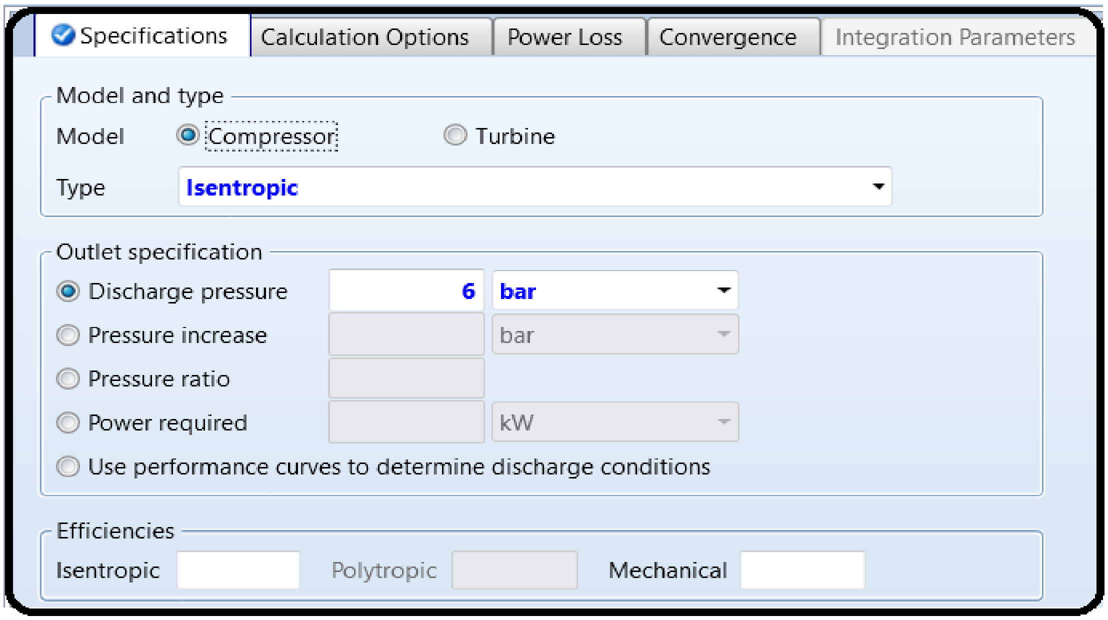
Figure 14.22 shows the solid inlet stream properties in terms of *P*, *T*, compositional flowrate, and PSD



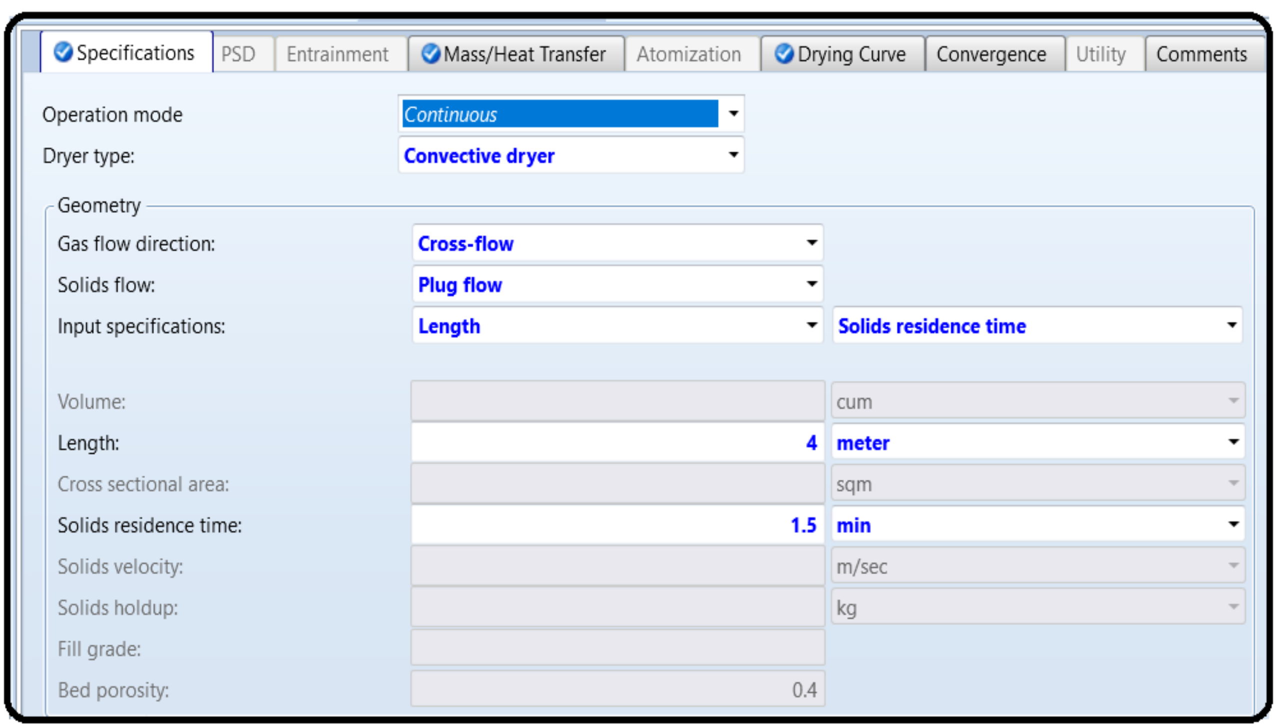
The inlet air stream enters the compressor at a flow rate of 3000 kg/h at room temperature and pressure and will leave it at 6 bar. The dryer specifications are shown in Figure 14.23.



5.Click Next to go to Compressor Block.



Notice that the “**Shortcut**” is simpler than the “**Convective dryer**” method in terms of inputrequirements, nevertheless, less rigorous. The drying curve characteristics are shown in Figure 14.24. Notice that the **critical solids moisture content** is the moisture content at which further evaporation is mass-transfer limited and the second drying phase begins, and the **equilibrium solids moisture content** is the ultimate moisture content at which point no further drying is possible.



Results

Summary	Balance	Evaporation	Profiles	Evaporation Rate	Utility Usage	Status

Exhaust gas temperature	276.304908	C
Calculated duty	1.4428e-08	Gcal/hr
Solids residence time	0.025	hr
Solids velocity	0.0444444	m/sec
Critical moisture content (dry)	0.0526316	
Equilibrium moisture content (dry)	0.0309278	
Initial solids moisture content (dry)	0.25	
Outlet solids moisture content (dry)	0.0309278	
Overall evaporation rate	17.5258	kg/hr
Initial inlet vapor moisture content (dry)	0	
Outlet vapor moisture content (dry)	0.00584192	
Vapor temp at adiabatic saturation	53.9143	C
Vapor moisture content at adiabatic saturation	0.109343	
Calculated Lewis number	0.805167	
Calculated heat transfer coefficient	1502.07	kcal/hr-sqm-K

Material	Heat	Load	Vol.% Curves	Wt. % Curves	Petroleum	Polymers	Solids

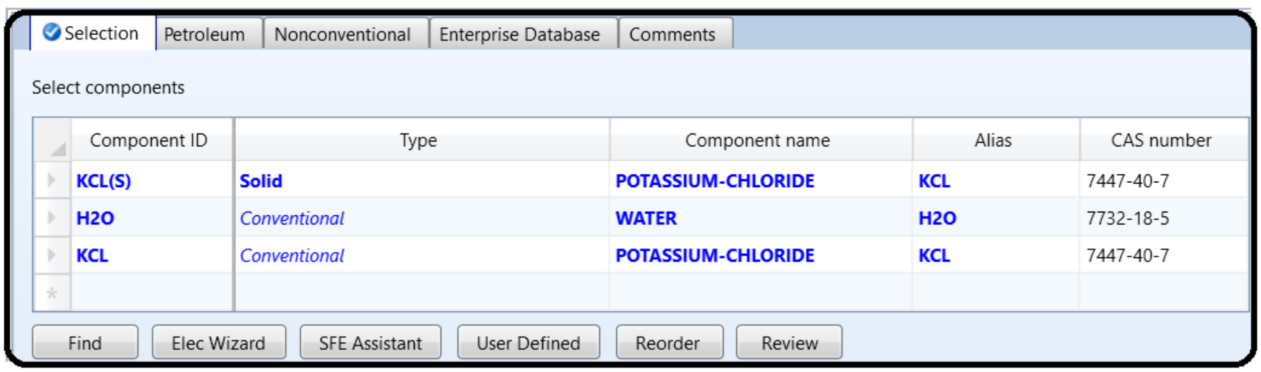
	Units	CA	SI	AO	SO
Mass Density	kg/cum	3.65269	1656.38	0.631502	1835.84
Enthalpy Flow	Gcal/hr	0.19935	-0.187651	0.128439	-0.116741
Average MW		28.9509	45.8031	28.8492	68.1362
+ Mole Flows	**kmol/hr**	**103.624**	**2.18326**	**104.597**	**1.21043**
+ Mole Fractions					
− Mass Flows	**kg/hr**	**3000**	**100**	**3017.53**	**82.4742**
KCL	kg/hr	0	80	0	80
AIR	kg/hr	3000	0	3000	0
H2O	kg/hr	0	20	17.5258	2.47423
+ Mass Fractions					
Volume Flow	cum/hr	821.313	0.0603725	4778.33	0.0449245

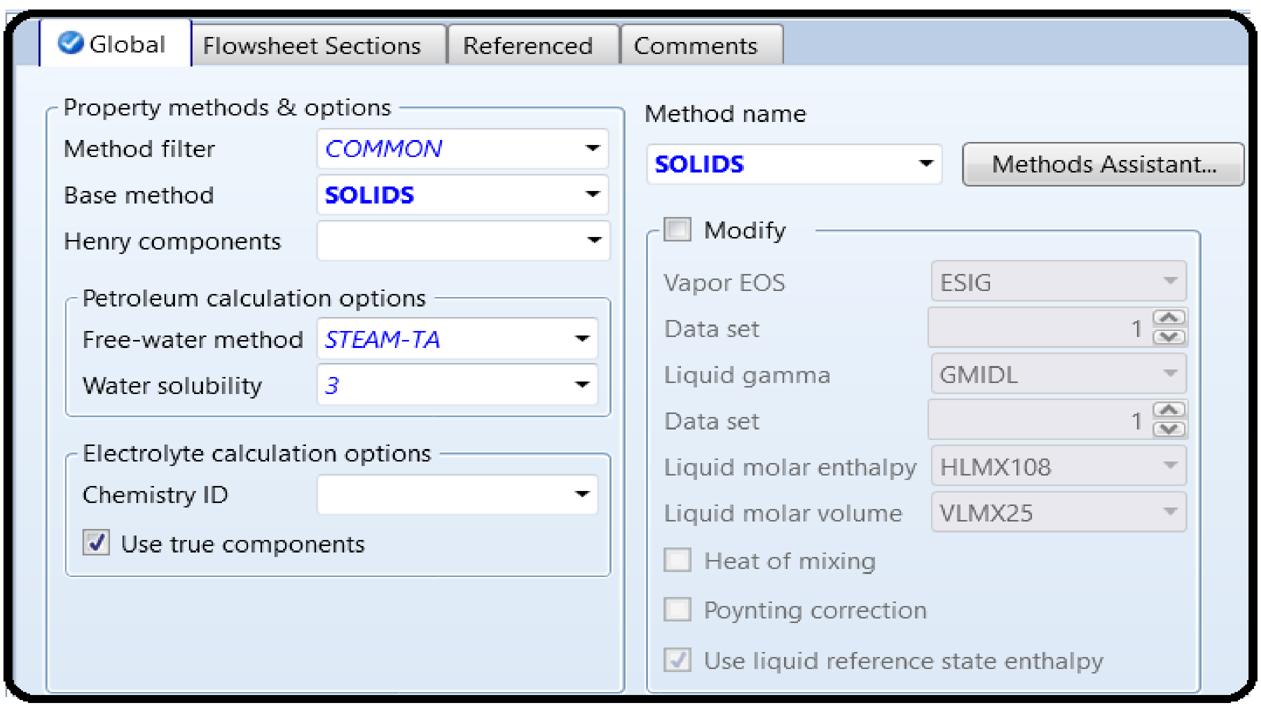
Part 4

<u>Example:</u> KCL CRYSTALLIZATION

Consider the process of KCl crystallization from KCl solution using heat to evaporate the water and result in a supersaturated solution that will be the cause for solid precipitation at the bottom of the mother liquor.

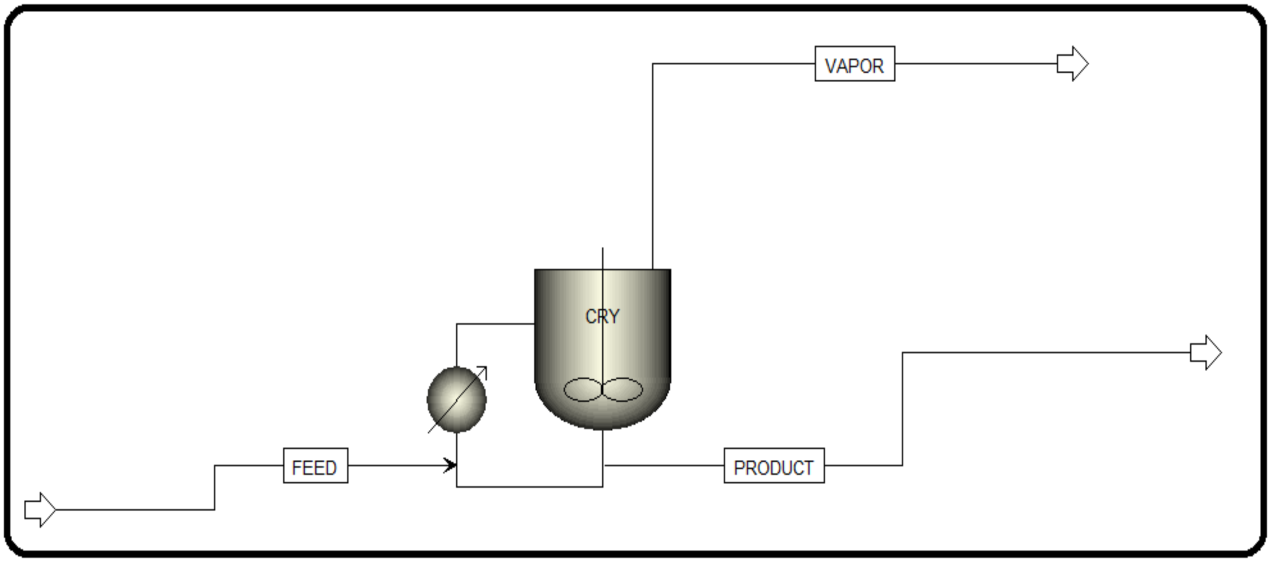
1. Using Aspen Plus, start a new simulation by choosing the “Solids” category and selecting “Solids with Metric Units” template to create a steady-state flowsheet. Notice that Aspen Plus does not assign a default property method. So, we will set it to “SOLIDS”.
2.In “Navigation” pane menu tree, go to “Components” | “Specifications” | “Selection” sheet. Add KCl twice once as “*Solid*” (i.e., “KCL(S)”) and another as “Conventional” (i.e., “KCL”) to the list of components and add water as well, as shown in Figure 14.25.



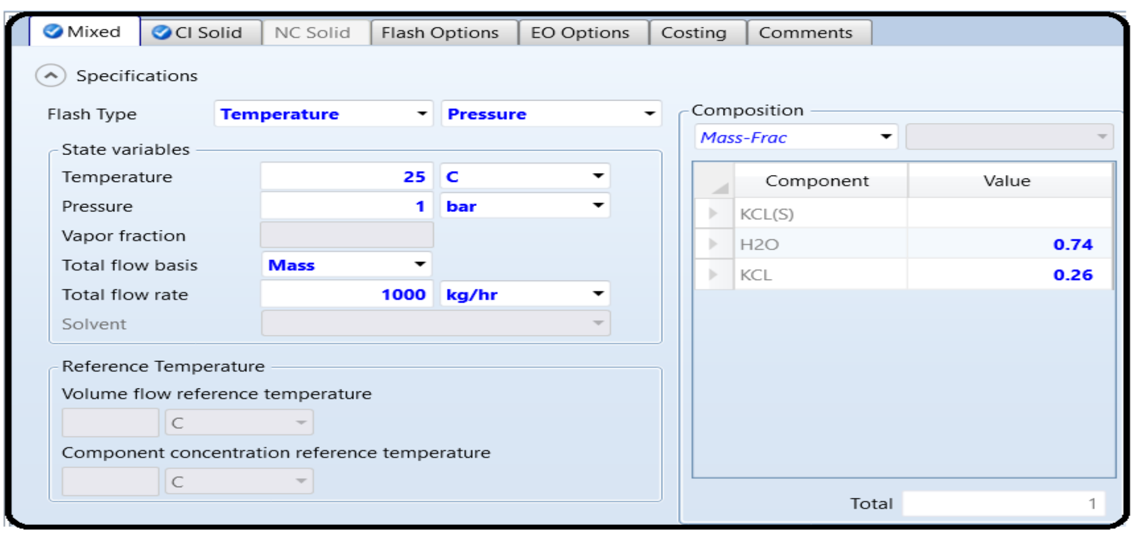


3. Click on “Next” button, run the simulator, and monitor warning and errors (if any) via the “Control Panel”. Once you successfully manage to complete the property analysis step, switch to “Simulation” environment.

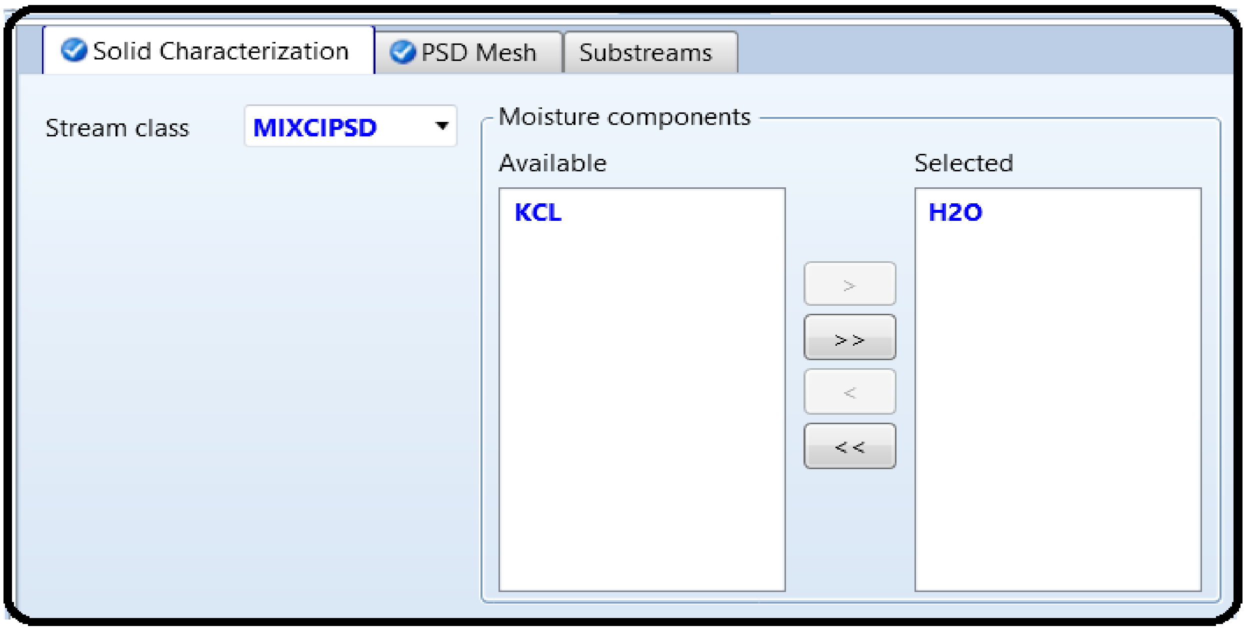
4.From “Model Palette”, select “Solids” tab, click on “Crystallizer” icon, and add the crystallizer icon to the flowsheet area. In addition, add the proper input and output streams, as shown in Figure 14.26.



5.Figure 14.29 shows the feed stream properties in terms of *P*, *T*, and compositional flowrate. There will be no need for PSD specification because the feed stream is a saturated aqueous KCl solution entering at the maximum solubility, which is 35 g KCl/100 g water (amounts to KCl mass fraction of 0.26).



Under “**Solids**” folder, selectwater as the moisture component, as shown in Figure 14.27.



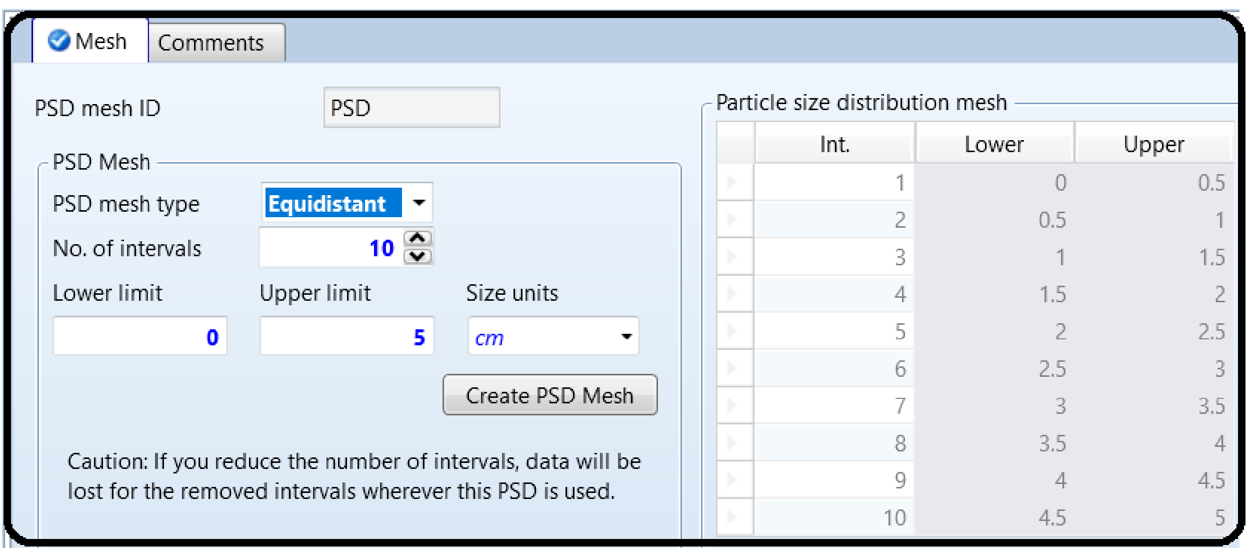
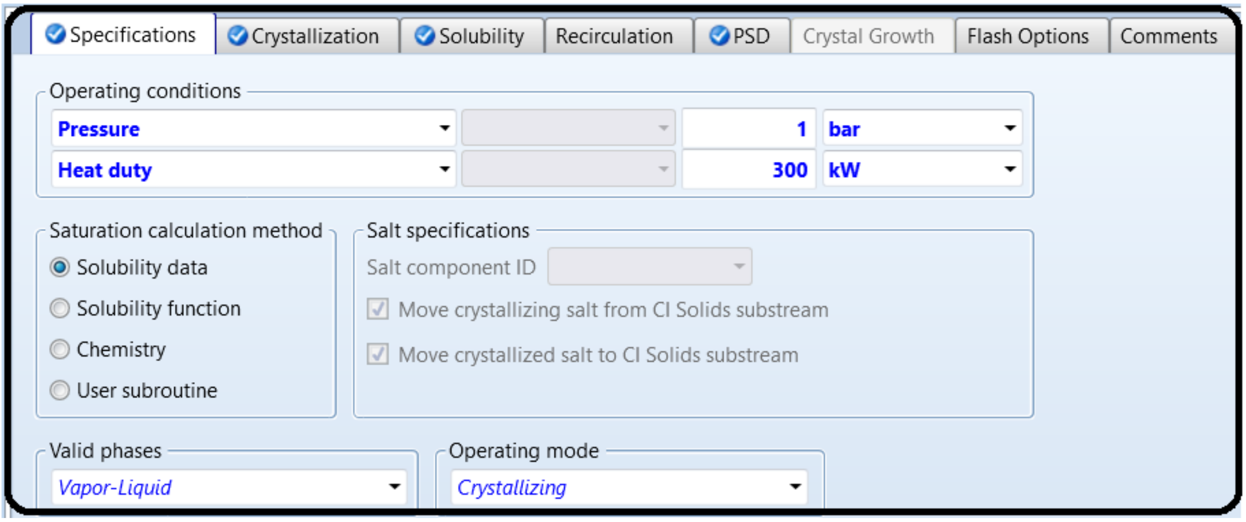


Figure 14.30 shows the “**Specifications**” tab window for the crystallizer. A heat duty of 300kW will be supplied to evaporate water (the solvent) and concentrate KCl solution. The “**Operating mode**” is set to “*Crystallizing*”. Under this mode, the amount of crystals should increase in the flow and a warning will be issued if the crystal product flow rate iszero or smaller than that of the inlet. The opposite is true for the “*Dissolving or melting*” mode. No warning will be issued if the

mode is set to “*Either*”. Figure 14.31 shows the “Crystallization” tab window where we define the sort of speaking “physical” reaction:KCl(aq) → KCl(S).



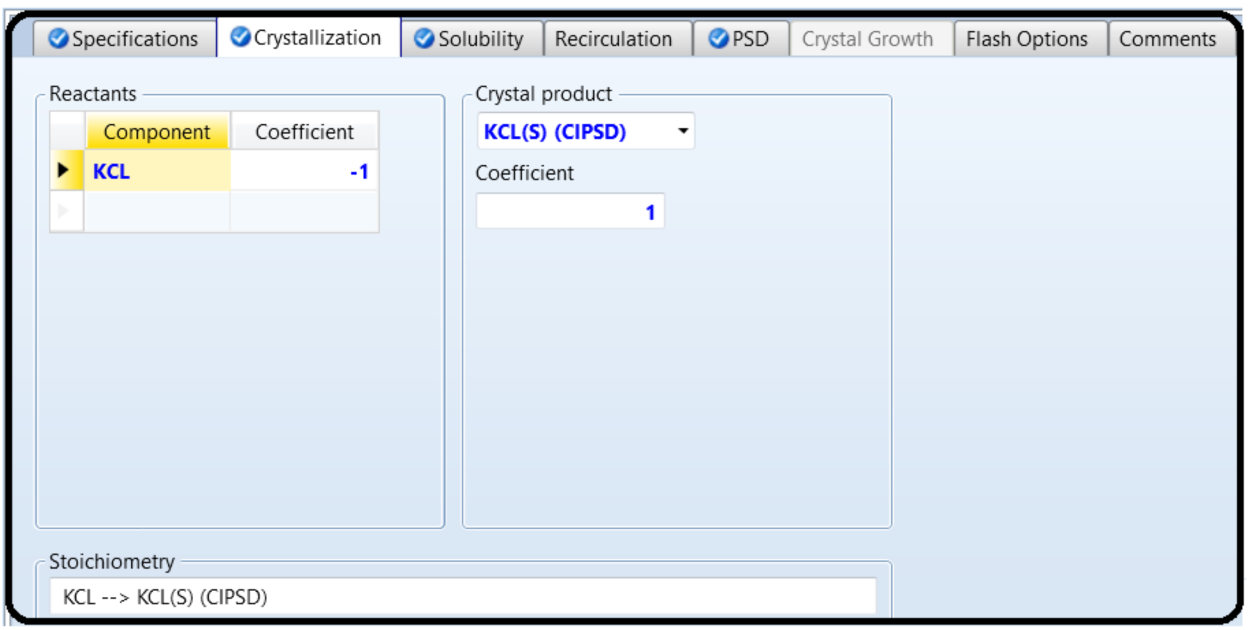


Figure 14.32 shows the “Solubility” tab window where we enter the solubility data for KCl in water at room temperature. In the literature, it is reported as 35 g KCl per 100 g H2O.

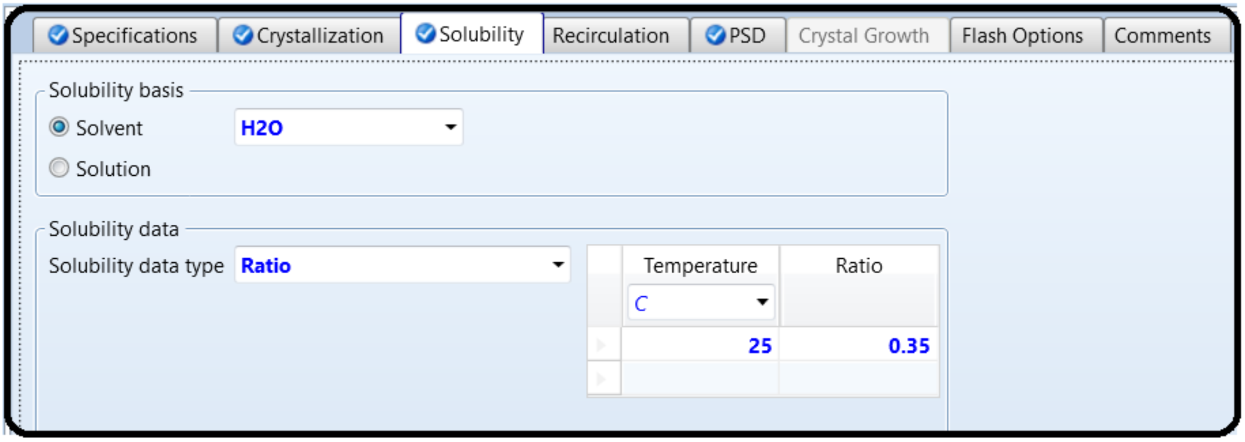
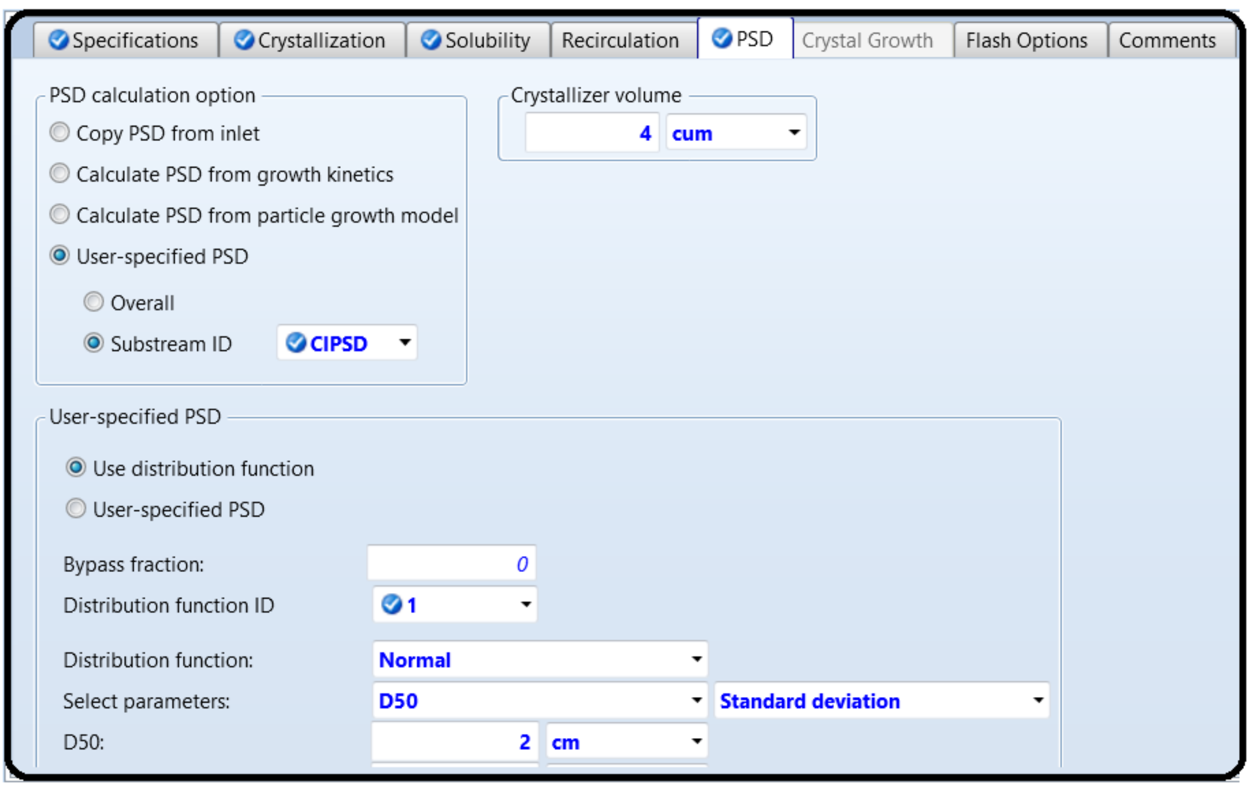


Figure 14.33 shows the “**PSD**” tab window where the outlet PSD is defined in terms of a built-in known distribution function; namely, the normal distribution.



Results

Summary		
Crystallizer temperature	101.937	C
Heater duty	300	kW
Net duty	0	Gcal/hr
Crystallizer pressure	1	bar
Crystallizer volume	4	cum
Residence time	7.80996	hr
Crystal product	133.127	kg/hr
Vapor flow rate	377.506	kg/hr
Recirculation flow rate	0	kg/hr
Magma density	259.928	gm/l

	Units	FEED	PRODUCT	VAPOR
Temperature	C	25	101.937	101.937
Pressure	bar	1	1	1
Molar Vapor Fraction		0	0	1
Molar Liquid Fraction		1	0.924363	0
Molar Solid Fraction		0	0.0756368	0
Mass Vapor Fraction		0	0	1
Mass Liquid Fraction		1	0.78614	0
Mass Solid Fraction		0	0.21386	0
Molar Enthalpy	kcal/mol	-70.7673	-71.9398	-57.1363
Mass Enthalpy	kcal/kg	-3153.66	-2728.42	-3171.55
Molar Entropy	cal/mol-K	-37.5682	-32.1967	-8.73304
Mass Entropy	cal/gm-K	-1.67418	-1.22111	-0.484757
Molar Density	mol/cc	0.0509796	0.0460964	3.20657e-05
Mass Density	kg/cum	1143.97	1215.41	0.577673

Appendix

Unit operations models used to describe treatment steps carried out on solids in the form of formation, size modification, size-based separation, washing, drying, and fluidization. Aspen Plus built-in unit operation solid models are

1. Crystallizer: produces crystals from solution based on solubility.
2. Crusher: breaks down solid particles to a smaller size.
3. Screen: separates solid particle based on their particle size.
4. Swash: separates solid particles from an entrained liquid of a solids stream using a washing liquid.
5. CCD: separates solid particles from an entrained liquid of a solids stream using a washing liquid in a countercurrent decanter or a multistage washer.
6. Dryer: evaporates volatile moisture components from wet solids.
7. Spray Dryer: evaporates moisture to form particles from sprinkled droplets.
8. Granulator: increases the size of solid particles.
9. Classifier: separates solid particles based on settling velocity.
10. Fluidized Bed: considers both chemical reactions and fluid mechanics.

Solids Separators Models

Unit operation models for separating solids from gases and/or liquids are shown in Table 14.A.1.

TABLE 14.A.1 Unit Operation Models for Solid/Liquid and/or Solid/Gas Separation.

Model	Description	Purpose	Use For
Cyclone	Cyclone separator	Separates solids from gas using gas vortex in a cyclone	Rating and sizing cyclones
VScrub	Venturi scrubber	Separates solids from gas by direct contact with an atomized liquid	Rating and sizing venturi scrubbers
CFuge	Centrifuge filter	Separates solids from liquid using a rotating basket	Rating or sizing centrifuges
Filter	Rotary vacuum filter	Separates solids from liquid using a continuous rotary vacuum filter	Rating or sizing rotary vacuum filters
HyCyc	Hydrocyclone	Separates solids from liquid using liquid vortex in a hydrocyclone	Rating or sizing hydrocyclones
FabFl	Fabric filter	Separates solids from gas using fabric filter baghouses	Rating and sizing baghouses
ESP	Electrostatic precipitator	Separates solids from gas using an electric charge between two plates	Rating and sizing dry electrostatic precipitators

Solids Handling Models

Pneumatic conveyance of granular solid materials over short and long distances through pipes. This includes solids transport through a single pipe or pipeline network.

SOLIDS CLASSIFICATION

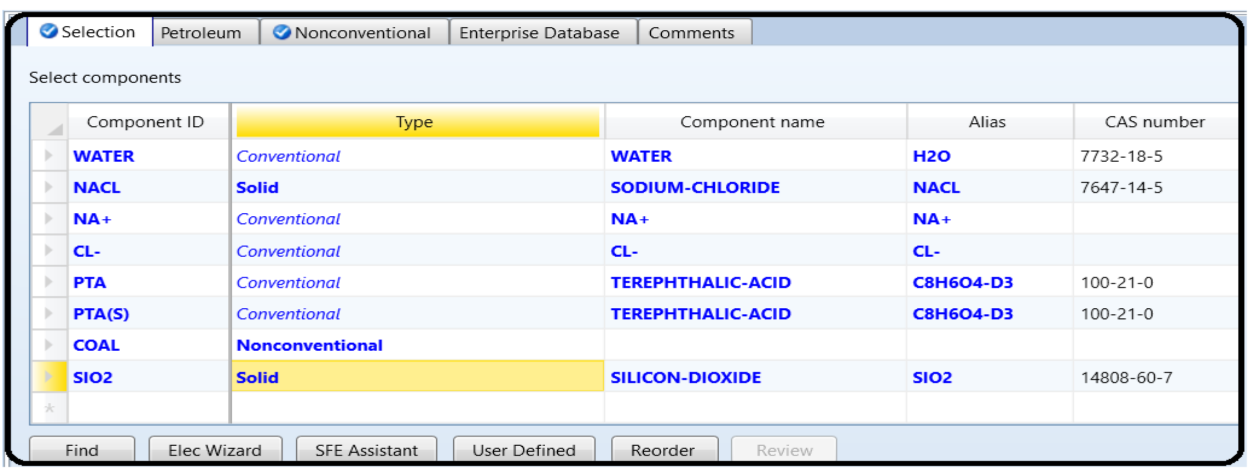
Solids are classified by Aspen Plus as shown in Table 14.B.1.

TABLE 14.B.1 Solids Classification Based on Knowledge of Molecular Structure and Chemical Reactivity.

Class	Type	Characteristics	Example
Conventional (a solid with a well-defined molecular structure)	Salts	Participates in phase equilibrium thus defined through chemistry	NaCl(s), ice, and purified terephthalic acid (pTA(s))
	Conventional Inert Solids (CISOLIDS)	An inert solid phase and does not participate in phase equilibrium	SiO_2(s) and urea(s)
Non-conventional (complex structure)	Non-conventional Solids (NCSOLIDS)	Characterized through component attributes (ultimate analysis) - special thermodynamic models	Coal and paper pulp

Figure 14.B.1 shows how one can define the same component using different types; hence, a different "Component ID" will be created each time. For example, if "NACL" is defined as "*Conventional*", then it will be part of the aqueous medium (i.e., participates in phase equilibrium); on the other hand, if it is defined as "NACL(S)", that is, "*Solid*", then it will be treated as inert (i.e., will not be part of the aqueous medium). Silica being defined as "*Solid*" means it is with a known molecular structure; on the other hand, coal being defined as "*Nonconventional*" means that it has a complex structure.

PREDEFINED STREAM CLASSIFICATION


Selection | Petroleum | Nonconventional | Enterprise Database | Comments

Select components

Component ID	Type	Component name	Alias	CAS number
WATER	Conventional	WATER	H2O	7732-18-5
NACL	Solid	SODIUM-CHLORIDE	NACL	7647-14-5
NA+	Conventional	NA+	NA+	
CL-	Conventional	CL-	CL-	
PTA	Conventional	TEREPHTHALIC-ACID	C8H6O4-D3	100-21-0
PTA(S)	Conventional	TEREPHTHALIC-ACID	C8H6O4-D3	100-21-0
COAL	Nonconventional			
SIO2	Solid	SILICON-DIOXIDE	SIO2	14808-60-7

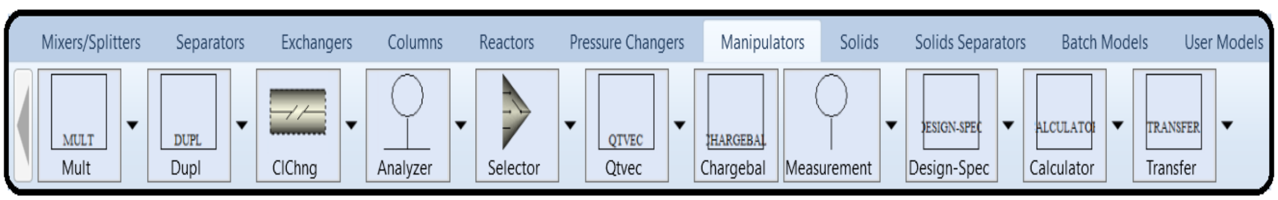
Find | Elec Wizard | SFE Assistant | User Defined | Reorder | Review

Stream classes are very useful when modeling solids because they can be used to differentiate between the properties of each substream in the simulation. Stream classes ease the integration of solids and fluids in one simulation. The stream class can either be created or selected from a predefined type. Upon one's need, a predefined class can also be modified. Aspen Plus predefined stream classes are in general sufficient for most applications. All unit operation models, except "Extract", can handle stream classes with solid substreams. Table 14.C.1 shows different Aspen Plus built-in stream classes.

TABLE 14.C.1 Aspen Plus Built-In Stream Classes.

Stream Class	When
CONVEN	The simulation does not involve solids, or the only solids are electrolytes salts
MIXCISLD	Conventional inert solids are present, but there is no particle size distribution
MIXNC	Non-conventional solids are present, but there is no particle size distribution
MIXCINC	Both conventional inert and non-conventional solids are present, but there is no particle size distribution
MIXCIPSD	Conventional inert solids are present, with a particle size distribution
MIXNCPSD	Non-conventional solids are present, with a particle size distribution

The stream class can be changed to a different class using the stream class changer (manipulator) as shown in Figure 14.C.1.



SUBSTREAM CLASSES

Substream classes are the building blocks of stream classes. They can either be predefined or customized. Predefined substream classes are shown in Table 14.D.1:

TABLE 14.D.1 Substream Classes for Solid-Bearing Streams.

#	Substream Class	Description
1	MIXED	Fluids only
2	CISOLID	Conventional inert solids that participate in reactions but do not participate in phase equilibria (except in the RGibbs model)
3	NC	Non-conventional solids
4	NCPSD	Non-conventional solids with PSD
5	CIPSD	Conventional inert solids with PSD

Notice that PSD can be specified for each substream in a stream class. Such an advantage permits the user to have different PSD functions for different streams or flowsheet sections. On the other hand, customized substream classes are additional substream types that can be created by the user to complement the existing predefined substreams. Customized substreams are usually used to ease the treatment of different solids in one simulation and permit the use of different PSDs for one predefined substream type, as shown in Figure 14.D.1.

PARTICLE SIZE DISTRIBUTION (PSD)

In Aspen Plus, particle size distribution (PSD) is represented by the weight fractions per particle size interval, given the number of intervals and the size range for each interval. In other words, a PSD describes the amount of particles in a sample of material with respect to size. The built in Aspen Plus particle size distribution has 10 predefined size intervals. The user can modify the built in particle size distribution by changing the number of intervals or the size ranges for the intervals. In some situations, he/she may want to have two or more particle size distribution definitions, with different size ranges. This will be useful if different sections of the flowsheet have different particle sizes. In this regard, a PSD mesh is defined (i.e., a grid with size intervals over which the particle sizes will be described). The PSD is populated via experimental results (i.e., user-specified weight fractions) or utilizing built-in distribution functions. In Aspen Plus, there are simulation PSD meshes coined for a substream under which all the results for multiple streams will be presented and input stream PSD meshes that are defined for individual feed streams. For user-specified PSD meshes, Aspen Plus provides four types: equidistant, geometric, logarithmic, and user-defined, where the user is required to enter the lower limit, upper limit, and size unit (i.e., mm, μm, angstrom, etc.). Depending on the selected type, the user may also have to enter the number of intervals. For the user-defined type, it is suited for experimental data where the user can copy and paste values from other spreadsheet packages such as Microsoft Excel sheet.
For built-in distribution functions, the user, however,must specify the function parameters that describe, in general, the mean or a reference datum and the degree of scatter around that mean or reference value, as in the following distributions:

1. Gates–Gaudin–Schuhmann (GSS): It has two parameters: one for the maximum particle size (i.e., at which the cumulative mass fraction *Q*(*d*)=*1*) and another for describing the profile (shape) of the distribution itself (i.e., narrow vs. broad). GGS is suited for coarse grinding.

2. Rosin–Rammler–Sperling–Bennet (RRSB): It has two parameters: one for the particle size (i.e., at which the cumulative mass fraction *Q*(*d*)=*0.632*) and another for describing the profile of the distribution itself (i.e., narrow vs. broad). RRSB is suited for fine grinding.

3. Normal: It has two parameters: one for the mean or median (at which the cumulative mass fraction *Q*(*d*)=*0.5*) and another for describing the profile of the distribution itself (i.e., narrow vs. broad).

4. Log Normal: It has two parameters: one for the median (the median at which the cumulative mass fraction *Q*(*d*)=*0.5*) and another for describing the profile of the distribution itself (i.e., narrow vs. broad). If particles are broken up at random, they will end up with such a distribution.
When viewing and analyzing the results for solid components, Aspen Plus provides sets of properties:

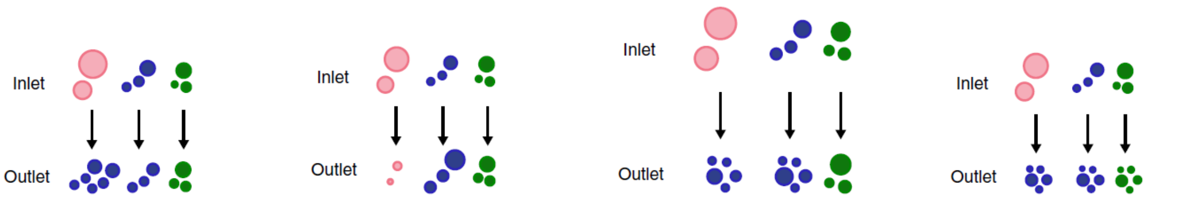
1. Median value (D50): the size at which 50% of particles are larger.
2. Mean particle size (D1_0): the sum over all intervals for the multiplication of the average particle size, in one interval, by the fraction.
3. Specific surface area (VSSA): the ratio of the surface area of a particle to its volume. For a completely spherical object, it is $4\pi r^2/\frac{4}{3}\pi r^3 = \frac{3}{r} = \frac{6}{D}$. For other non-spherical objects, a shape or sphericity factor is used.
4. Sauter mean diameter (D3_2 or SMD): an average particle size. SMD is the diameter of spheres with the same volume/area ratio as the particle mixture. For example, if *V* is the total volume of particles and *A* is their total surface area, then *SMD=6V/A=Dparticle*. SMD is inversely proportional to VSSA. SMD is the characteristic diameter for a packed bed flow and is mainly used in fluidized bed calculations.

FLUIDIZED BEDS

The Aspen Plus fluidized bed model describes a bubbling or circulating fluidized bed and tackles five different aspects: Entrainment of Particles: It takes into account the geometry of the vessel and additional gas supply and provides options to determine the minimum fluidization velocity, transport disengagement height, and distributor pressure drop for either a porous plate or bubble cap.
Chemical Reactions: After defining the reaction stoichiometry and its kinetics, the calculation method treats the gas as plug flow, the solids ideally mixed, and each balance cell is considered as CSTR (i.e., uniform in properties).
Fluid Mechanics: It assumes one-dimensional fluidmechanics and considers the impact of volume production/or reduction and heat exchange on fluid mechanics. Change in PSD: Table 14.F.1 demonstrates different options of tackling the outlet PSD with respect to the inlet PSD.

Thermodynamics: Solids and vapors are in thermodynamic equilibrium while the model considers the impact of heat exchange and heat effect on bed temperature.

TABLE 14.F.1 Different Approaches in Tackling the Outlet PSD For a Fluidized Bed.



Keep PSD	Constant # of Particles	Overall PSD	PSD Per Particle Type
Particle types have the same PSD as the inlet and the new generated particle types have the overall PSD from the inlet. Total number of particles may change and inert particles will keep the same size	Total number of particles is fixed. The particle may shrink or grow, depending on the mass loss/gain of the particle type. Inert particles will keep the same size	Overall bed PSD is defined by the user. Total number of particles may change. Inert particles are allowed to change their size	Bed PSD is defined by the user on a particle-type basis. Total number of particles may change. Inert particles will keep the same size if PSD is defined only for the reacting species

Reaction: A → B

Inert: C

The Aspen Plus fluidized bed model treats the bed as made of two zones. See Figure 14.F.1.

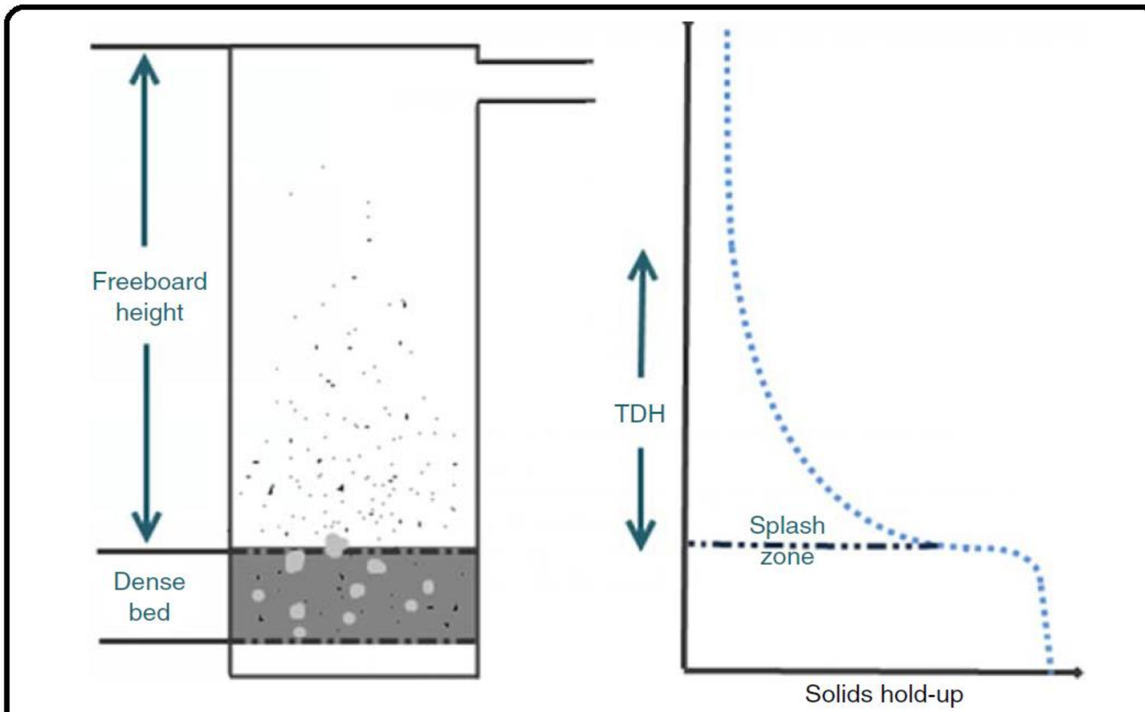


Figure 14.F.1 The fluidized bed is split into two zones the dense bed and the loose bed (freeboard). TDH stands for transport disengagement height.

The bottom zone (dense bed): High solids concentration and fluid mechanics is dealt with according to Werther and Wein [1], which considers the growth and splitting of bubbles. Bubble-related profiles (e.g., bubble diameter, bubble rise velocity, interstitial gas velocity, pressure, and solid volume concentration profiles can all be calculated.

The freeboard zone (loose bed): Relatively low solids concentration and fluid mechanics is dealt with according to Kunii and Levenspiel [2]. Using the selected entrainment correlation, the solids mass flow and PSD at the outlet condition can be calculated. Overall, once the user defines bed inventory, by specifying the pressure drop or the solids hold-up, the height of the bottom zone and the freeboard can be determined.

Reference

1. Our team experience

2. Werther, J. and Wein, J. (1994) Expansion behavior of gas fluidized beds in the turbulent regime. AIChE Symposium Series, **90** (301), 31–44.

3. Kunii, D. and Leven spiel, O. (1991) Fluidization Engineering, Butterworth-Heinemann, Boston.

4. Aspen Plus – Chemical Engineering Application by KAMAL I.M. AL-MALAH