

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.





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. 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		Туре			Component na	ame	Alias	CAS number		
Þ	KCL	Solid			POT	ASSIUM-CHLORIE	DE	KCL	7447-40-7		
*											
\bigcap	🥝 Global	Flowsheet	Sections	Referenced		Comments					
	Property me	thods & c	ptions —			Method nam	e				
	Method filte	er	COMMON	-	•	SOLIDS		 Method 	ds Assistant		
	Base metho	d	SOLIDS	•	·	—)		
	Henry comp	onents		-		Modify					
	Petroleum	calculatio	n options -			Vapor EOS		ESIG	-		
	Free-water	r method	STEAM-TA	•		Data set			1		
	Water solu	bility	3	•		Liquid gam	ma	GMIDL	-		
						Data set			1		
	Electrolyte	e calculatio	on options -			Liquid mola	ar enthalpy	HLMX108	-		
	Chemistry	ID		•		Liquid mola	ar volume	VLMX25	-		
	Use true components					📃 Heat of	mixing				
						Poynting	g correctio	n			
l						Use liquid reference state enthalpy					

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.

\bigcap	🕑 Mixed	⊖Cl Solid	NC Solid	Flash (Options	EO Options	Costing	Comment	s			
(.	Specific	ations									•	Component Attribute
	State vari	ables]	Compo	sition ——				Particle Size Distribution
	Substream	n name	CIPSD			•	Mass-I	rac	•	~		
	Temperat	ture		20	C	•		Component		Value		
	Pressure			1	bar	•	KCI	-		1		
	Total flov	v basis	Mass	•								
	Total flov	v rate		1250	kg/hr	•		То	tal	1		
)	

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.

	🥑 FI	owsheet	Streams	Stream Class	Load Streams	Comments
	Def	ine stream	class for flo			
	Sectio		on	Stream class		
l	►	GLOBAL	М	XCIPSD		

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	S Flowsheet	Streams	0	Stream Class	Load Streams	Comments		
S	Stream class MIXCIPSD							
	CISOLID NC NCPSD		>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>	ASS MIXED CIPSD				

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.

Mesh Comm	ents										
PSD mesh ID	PSD		Par	Particle size distribution mesh							
- PSD Mesh				Int.	Lower	Upper					
PSD mesh type	Fauidistant -			1	0	1					
PSD mesh type	Equiuistant			2	1	2					
No. of intervals	10 👻			3	2	3					
Lower limit	Upper limit	Size units		4	3	4					
0	10	mm 🔻	►	5	4	5					
			•	6	5	6					
		Create PSD Mesh		7	6	7					
Caution If your	aduce the number of i	atanyala data will be		8	7	8					
lost for the rem	oved intervals whereve	er this PSD is used.	•	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.

0	Mixed	🕑 CI Solid	NC Solid	Flash Options	EO Options	Costing	Comments									i
							•	Component Attribute								
				Composition -				Particle Size Distribution	ı							
IPSD			•	Mass-Frac	•		- P	SD mesh ID	▼ Units	mm		Interval	Lower limit	Unner limit	Weight fraction	Cumulative
	20	c	•	Compo	nent	Value			onito			interval	LOWCI IIIII	opper mine	meight nuction	weight fraction
	1	bar	-	KCL			1			Edit PSD	Mesh	1	0	1	3.1686e-05	3.1686e-05
_	_							Populate PSD using				2	1	2	0.00131828	0.00134997
5	•							User-specified values				3	2	3	0.0214001	0.0227501
	1250	kg/hr	•		Total		1	A distribution function				4	3	4	0.135905	0.158655
								© A distribution function				5	4	5	0.341345	0.5
								Distribution function				6	5	6	0.341345	0.841345
								Туре	Normal	•		7	6	7	0.135905	0.97725
								Standard deviation		1 mm	•	8	7	8	0.0214001	0.99865
								D50	_	5 mm	-	9	8	9	0.00131828	0.999969
								050		2 1000		10	9	10	3.13989e-05	1
-										Calcu	ulate					

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

Specif	ications	Grindability	Selection Functio	n Brea	kage Functio	n Utility	Com	ments				
COutlet PS	SD calcula	ation method: –										
Select	equipme	ent										
O Deter	mine out	let PSD from co	mminution power	and a dis	tribution fund	tion						
🔘 Speci	Specify outlet PSD											
Operatin	a parame	eters										
Crusher t	ype			Gyratory	,				-			
Selection	Selection function:				US Bureau of Mines -							
Breakage	e function	:		US Burea	u of Mines				•			
Distribut	ion functi	on:		Rosin Rai	mmler Sperlir	ng Bennet			-			
Selection	n function	parameters —										
Operatin	g mode			Primary	•							
Brookage	function	parameters										
Mavir	num part	icle diameter			2	mm	•					
	specific:	ation			-	kW.	-					
© Speci	fic nower					kWhr/top						
Ratio of	cut-off size	ze to solids outl	et diameter		1.7	KWIII/ toll						

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		
C. L. L. L. L				4 47070000 - 20	
Calculated p	ower			1.17070888e-30	KVV 🗸
Particle dian than 80% of	neter which inlet mass	is larger		0.00587888	meter 🝷
Particle dian than 80% of	neter which outlet mass	is larger		0.00183233	meter 👻
Particle dian than 50% of	neter which inlet mass	is larger		0.005	meter 💌
Particle diam	neter which	is larger			
than 50% of	outlet mass	s		0.00088407	meter 🝷
Size reduction	on ratio of [080		3.20841	
Size reduction	on ratio of [050		5.65566	
Sauter mean	diameter o	of inlet particles		0.00475806	meter 🔹
Sauter mean	diameter o	of outlet particles		0.000725362	meter 🝷



ſ	Material	Work	Vol.% Curves	Wt. % Curves	Petroleum	Polyme	rs Solids		
					Units				
					Units		FEED	•	PRODUCT -
) + N	/lass Fra	ctions						
	▶ V	/olume F	low		cum/hr		0.628	824	0.628824
	▶ — P	SD							
	•	0 - 1	mm				3.16866	e-05	0.565566
	•	- 2 1	mm				0.00131	828	0.281658
	•	-3 1	mm				0.0214	001	0.140593
	•	- 4 1	mm				0.135	905	0.0121827
	•	- 5 1	mm				0.341	345	0
	•	-61	mm				0.341	345	0
	•	-7 1	mm				0.135	905	0
	•	- 8 1	mm				0.0214	001	0
	•	-91	mm				0.00131	828	0
	•	- 10	mm				3.13989e	e-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 🖉	
Coloriated				
Calculated	power		1	kW 👻
Particle dia than 80% c	meter which of inlet mass	is larger	0.00587888	meter •
Particle dia than 80% c	meter which of outlet mas	is larger s	0.0016	meter -
Particle dia than 50% c	meter which of inlet mass	is larger	0.005	meter -
Particle dia than 50% c	meter which of outlet mas	is larger s	0.000999989	meter -
Size reduct	ion ratio of l	280	3.67431	
Size reduct	ion ratio of l	D50	5.00006	
Sauter mea	n diameter o	of inlet particles	0.00475806	meter -
Sauter mea	in diameter o	of outlet particles	0.000749996	meter 🝷

Material	Work	Vol.% Curves	Wt. % Curves	Petroleum	Polyme	rs Solids		
				Units		FEED	T	PRODUCT -
) + M	/lass Fra	ctions						
> V	/olume F	low		cum/hr		0.628	824	0.628824
> - F	SD							
•	0 - 1	mm				3.1686e	-05	0.500006
•	-21	mm				0.00131	828	0.499994
•	-3 r	mm				0.0214	001	0
	-4 1	mm				0.135	905	0
•	- 5 r	mm				0.341	345	0
•	-6 I	mm				0.341	345	0
•	-7 r	mm				0.135	905	0
	- 8 1	mm				0.0214	001	0
•	-9 i	mm				0.00131	828	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.

Summary Balance	e Utility Usage	Status	
Calculated power		0.555457537	kW -
Particle diameter whi	ich is larger	0.00587888	meter -
than 80% of inlet ma	SS	0100001000	Incer
Particle diameter whi than 80% of outlet m	ch is larger 1ass	0.00187888	meter -
Particle diameter whi than 50% of inlet ma	ich is larger ss	0.005	meter -
Particle diameter whi than 50% of outlet m	ich is larger nass	0.001	meter 🝷
Size reduction ratio c	of D80	3.12893	
Size reduction ratio of	of D50	5	
Sauter mean diamete	er of inlet particles	0.00475806	meter -
Sauter mean diamete	er of outlet particles	0.000776194	meter 👻



Material	Work	Vol.% Curves	Wt. % Curves	Petroleum	Polyme	rs Solids		
				Units		FEED	•	PRODUCT -
► +	Mass Fra	ctions						
•	Volume F	low		cum/hr		0.628	824	0.628824
	PSD							
•	0 - 1	mm				3.16866	e-05	0.5
•	- 2	mm				0.00131	828	0.341345
•	- 3	mm				0.0214	001	0.135905
•	- 4	mm				0.135	905	0.0214002
•	- 5	mm				0.341	345	0.00131823
•	- 6	mm				0.341	345	3.13846e-05
•	- 7	mm				0.135	905	2.85665e-07
•	- 8	mm				0.0214	001	9.85308e-10
•	- 9	mm				0.00131	828	1.2792e-12
•	- 10	mm				3.13989€	e-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

 $\text{2AI (OH)3} \rightarrow \text{AI2O3} + \text{3H2O}$

can be put in another form:

 $\text{Al2O3} \cdot 3\text{H2O} \rightarrow \text{Al2O3} + 3\text{H2O}$

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

<u>1.</u> 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.

$\left(\right)$	0	Selection Petroleu	m Nonconventional Enterprise Database	Comments							
S	ele	ct components									
		Component ID	Туре	Component name	Alias	CAS number					
	Þ	AL(OH)3	Solid	ALUMINIUM-HYDROXIDE	AL(OH)3	21645-51-2					
	Þ	AL2O3	Solid	ALUMINIUM-OXIDE-ALPHA-C	AL2O3	1344-28-1					
	▶	AIR	Conventional	AIR	AIR	132259-10-0					
	Þ	WATER	Conventional	WATER	H2O	7732-18-5					
	*										
	Find Elec Wizard SFE Assistant User Defined Reorder Review										

Global F	lowsheet Sections	Referenced	Comments						
Property met	hods & options — COMMON	<i>I</i> -	Method name						
Base method Henry compo	soLIDS	•	Modify						
Petroleum o Free-water i Water solub	alculation options method <i>STEAM-TA</i> ility <i>3</i>	•	Vapor EOS Data set Liquid gamma	ESIG					
Electrolyte of Chemistry I	calculation options		Data set Liquid molar enthalpy Liquid molar volume	1 💌 HLMX108 🔍 VLMX25 🔍					
Use true	components		 Heat of mixing Poynting correction Use liquid reference 	e state enthalpy					



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*).



Ø Mixed	🕝 CI Solid	NC Solid	Flash (Options	EO Options	Costin	g	Comments		
Specif	ications									
Flash Type	e Tem	perature	•	Pressur	e ·		mp	osition —		
- State va	riables —						ass	-Frac	•	Ŧ
Tempera	ature		25	С	•			Component		Value
Pressure	•		1	bar	•			AL(OH)3		
Vapor fr	action							AL2O3		
Total flo	w basis	Mass	•					AIR		1
Total flo	w rate		4500	kg/hr	-		. 1	WATER		
Solvent					~					
Referen	ce Temperatur	e								
Volume	flow reference	temperature								
	С	-								
Compor	nent concentra	tion reference	tempe	erature						
	С	-								
								To	tal	1



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Specifications								 ♥ Component Attribute 			
tate variables —				Comp	osition —			Particle Size Distribution	1		
ubstream name	CIPSD		•	Mass	-Flow 🔻	kg/hr	•				
emperature	2!	5 C	T		Component	Value		PSD mesh ID PSD	 Units 	mm	
ressure	12	2 bar	•			Value	1			Edit P	SD M
tal flow basis	Mage			> A	L203			Populate PSD using			
	Widss		_		Tetel		4	O User-specified values			
otal flow rate	500	, kg/nr	•		Iotai			A distribution function			
								Distribution function			
								Туре	GGS	<u> </u>	
								Dispersion parameter	1.	5	
								Maximum diameter	1) mm	
										_	
										Ca	lcula



Mesh Commer	its					
PSD mesh ID	PSD		Particle	e size distributio	on mesh	
DSD Mach				Int.	Lower	Upper
PSD Wesh				1	0	1
PSD mesh type	Equidistant 👻		•	2	1	2
No. of intervals	10 🚭		•	3	2	3
Lower limit	Upper limit	Size units	•	4	3	4
0	10	mm 🔹	•	5	4	5
			•	6	5	6
		Create PSD Mesh	•	7	6	7
C .:			•	8	7	8
Lost for the remov	luce the number of it ed intervals whereve	rtervals, data will be r this PSD is used	•	9	8	9
lost for the remov	cu mervais whereve	1 1113 1 30 13 4304.	•	10	9	10

Specificat	ions	Calcula	ation Options	Power Lo	ss Converg	gence In	tegration Paramete	rs Utility	Comments
Model and t Model @	ype —) Con	npresso	r © T	urbine					
Туре	lsentr	opic					•		
Outlet specif	ficatio	n —							
Oischarge	e press	sure	12	bar	•				
Pressure i	increas	e		bar	Ŧ				
Pressure r	ratio								
Power rec	quired			kW	-				
🔘 Use perfo	ormano	e curve	s to determine	discharge	conditions				
Efficiencies									
Isentropic			Polytropic		Mechanical				

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 10mm 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	Geome	etry 🤇	Gas Distributo	r Heat I	Exchanger	Reactior	ns PSD	Converg	ence	Comments
	Bed inventory]
	Specify bed ma	ISS			120	kg		•				
	Specify bed pre	essure drop				bar		Ŧ				
	Voidage at minim	um fluidization			0.5							
	Geldart classificati	on		Geldart	В			•				
	- Minimum fluidizat	ion velocity —										
	Specify velocity	i veroenty		m/sec 👻								
	 Calculate from 	correlation		Ergun								
]
	Transport disenga	gement height —		C				_				
	Navimum dCu/db			George	Ina Grace			•				
	Elutriation				1e-05							
	Model		ſ	Tasirin 8	v Geldart			•				
	Docay constant			rustrario	- Getuart							
	Decay constant				3							
	TG parameter A1				$k_{i\cdot\infty} = A \cdot \rho_G \cdot u^B \cdot \exp\left(C - \frac{u_{t,i}}{u}\right)$							
	TG parameter A2				14.5				u ·			2
7	· · · · · ·						1			(-	
£	Specification	s 🔮 Operatio	on 🤍 🍼 Ge	eometry	/ Gas Di	stributor	Heat Excl	hanger 🤇	Reaction	is PSD	Co	nvergence
	Dimensions —											
	Height					4 meter -						
	Solids discharge	location			0.9	95						
	Cross-section			Cir	rcular			•				
	Constant dia	meter			0.	5 meter	•	•				
	🔘 Height-depe	ndent diameter	r									
	Width					meter		-				
	Depth	Depth				meter		-				
	- Height-depende	ent diameter							_			
	Location	Diamet	er									
		meter	-									
	>											
	Constant in the second											
	Secondary gas i	niet streams —										
	Name	Logation										



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Specifications Operation Operation	Gas Distributor H H H G H H G H G H G	eat Exchanger	Reactions	PSD	Convergence
Туре	Perforated plate		-		
Number of orifices	40 🖨				
Orifice diameter	10	mm	•		
Specify orifice discharge coefficient	0.8				
Specify distributor pressure drop		bar	T		
Number of bubble caps					
Number of cap orifices					
Cap orifice diameter		meter	v		
Specify cap orifice discharge coefficient	0.8				
O Specify distributor pressure drop		bar	T		

Specifications	Operation	Geometry	Gas Distributor	Heat Exchanger	Reactions	PSD	Convergence
Select reaction se	ts to be included i	n the model —		1			
Available reaction	n sets	Selected reacti	on sets				
		R-1					
	>						
	<						
	New						
				J			
Specifications	Operation	Geometry	Gas Distributor	Heat Exchanger	Reactions	PSD	Convergence
PSD calculation or	ption —						

Keep PSD

- Calculate PSD from particle growth model
- Our User-specified PSD



Specifications Operation Secondary	as Distributor Heat	Exchanger 🛛 🔗 Reaction	s PSD	Convergence
Convergence parameters				
Tolerance	0.0001			
Maximum number of iteration steps	100 🚭			
Number of cells for the bottom zone	100 🚭			
Number of cells for the dilute zone	100 🚭			
Bed mass threshold	1e-10			
Pressure drop threshold	1e-10			
Holdup convergence method	RootN1 -			
Pressure convergence method	RootN1 -			
C Flash options			_	
Tolerance	0.0001			
Maximum number of iterations	30 📚			
Temperature estimate		•		
Reaction convergence				
Mars balance convergence				
Solver	Newton	Newton Parameters		

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.

	0	Stoichiometry Stoichiometry		i c Equ	uilibriu	m Activity	Comments		
		New	Edi	it	Сор	y	Paste)	
		Rxn No.	Re	action t	ype	Stoich	iometry		Delete
l	Þ	1	Kinetio	с		2 AL(OH)3(CIPSD)	> AL2O3(CIPSD) + 3 WATER(MIXED)	×



•	Ed	lit Reaction									\times	
F	Reaction No. 🖉 1 🔹 Reaction type Kinetic 🔹											
ſ	Rea	ctants				Pro	oducts —					
		Component	Coefficient	Exponent			Compor	nent	Coefficient	Exponent		
	►	AL(OH)3 (CIPSD)	-2	1			AL2O3 (CI	IPSD)	1			
							WATER		3			
						►					T	
									IIII		•	
										Close		

Stoich	iometry	✓ Kinetic	Equilibrium	Activity	Comm	nents					
1) 2 AL(0	1) 2 AL(OH)3(CIPSD)> AL2O3(CIPSD) + 3 WATER(MIXED)										
Reacting p	hase	Vapor	-	Rate	basis	Reac ((vol) -				
Power La If To is s If To is n	Power Law kinetic expressionIf To is specifiedKinetic factor $=k(T/To)$ $n e^{-(E/R)[1/T-1/To]}$ If To is not specifiedKinetic factor $=kT$ $n e^{-E/RT}$										
k n			1 0				Solids				
E		2388.4	46 cal/mol		•						
То			С		•						
[Ci] basi	5	Molarity			•						



<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 cor	npositions 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	e 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 -



Ν	/laterial	Vol.% Curves	Wt. % Curves	Petrole	um	Polymers	Soli	ds					
	4					Units		CMPRSAIR	•	SIN 🔻	AIROUT -	SOUT -	
►	- Tota	l Stream											
Þ	1	Temperature			С			442.065	5	25	353.468	353.468	
Þ	F	ressure			bar			12	2	12	11.7259	11.7261	
Þ	Ν	Molar Vapor Frac	tion					1		0	0.999999	0	
Þ	Ν	Molar Liquid Frac	ction					C)	0	0	0	
Þ	Ν	Molar Solid Fract	tion					C)	1	5.92826e-07	1	
Þ	Ν	Mass Vapor Fract	ion					1	I	0	0.999998	0	
Þ	Ν	Mass Liquid Fract	tion					C)	0	0	0	
Þ	Ν	Mass Solid Fracti	on					C)	1	2.11621e-06	1	
Þ	Ν	Molar Enthalpy			kcal/	mol		2.97075	5	-304.767	0.267563	-391.763	
Þ	Ν	Mass Enthalpy			kcal/	kg		102.614	ļ	-3907.1	9.36854	-3842.71	
Þ	Ν	Molar Entropy			cal/mol-K		1.292	2	-96.9643	0.325636	-56.6278		
	Ν	Mass Entropy			cal/gm-K		0.0446271		-1.24308	0.0114019	-0.555448		
	Molar Density				mol/	cc		0.000201798	3	0.031024	0.00022507	0.0390551	



Part 3

Problem Definition: KCL DRYING

Consider the process of KCI 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.

0	25	Selection Petroleu	m Nonconventional Enterprise Database	Comments									
Sel	Select components												
		Component ID	Туре	Component name	Alias	CAS number							
	KCL		Solid	POTASSIUM-CHLORIDE	KCL	7447-40-7							
		AIR	Conventional	AIR	AIR	132259-10-0							
		H2O	Conventional	WATER	H2O	7732-18-5							
*													
	Find Elec Wizard SFE Assistant User Defined Reorder Review												

\bigcap	🥑 Global	Flowsheet	t Sections	Referenced	Comments								
	Property m	ethods & c	options —		Method nar	ne							
	Method filt	ter	COMMON	-	SOLIDS Methods Assistant								
	Base method SOLIDS				▼								
	Henry com	ponents		•	Modify	/							
	Petroleun	n calculatio	on options -		Vapor EOS	5	ESIG	~					
	Free-wate	er method	STEAM-TA	-	Data set			1 😴					
	Water sol	ubility	3	-	Liquid gar	mma	GMIDL	-					
					Data set			1 💌					
	Electrolyt	e calculatio	on options -		Liquid mo	lar enthalpy	HLMX108	-					
	Chemistry	/ ID		•	Liquid mo	lar volume	VLMX25	-					
	🔽 Use tr	ue compor	ents		🔲 Heat c	of mixing							
					🔲 Poyntii	ng correction							
					🔽 Use liq	uid reference	state enthalpy						

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.

Solid Chara	cterization	📀 PSD Mesh	Substreams			
Stream class	MIXCIPSD	Moi Ava	sture componen	ts	Selected	
		AI	R	>	H2O	
				<		

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.



Mesh Commen	ts						
PSD mesh ID	PSD		⊂ Pa	article	e size distribut	ion mesh ——	
DCD Mach					Int.	Lower	Upper
- PSD Wesh					1	1	1.4
PSD mesh type	Equidistant 🝷				2	1.4	1.8
No. of intervals	10 🚔				3	1.8	2.2
Lower limit	Upper limit	Size units			4	2.2	2.6
1	5	cm 🝷			5	2.6	3
					6	3	3.4
		Create PSD Mesh			7	3.4	3.8
Cautions If you and					8	3.8	4.2
Lost for the remove	uce the number of I ed intervals whereve	ntervais, data will be or this PSD is used			9	4.2	4.6
lost for the remov	cu intervals whereve	a this i se is used.			10	4.6	5

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

Mixed OCI Sol	id NC Solid	Flash Options	EO Options	Costing	Comments							
 Specifications 							 ✓ Component Attribute 					
State variables —				Composition			▲ Ø Particle Size Distribution					
Substream name	CIPSD		•	Mass-F	Mass-Frac 🔻				0.00			
Temperature		25 C	•		Component	Value	PSD mesh ID PSD	 Units 		cm		
Pressure		1 bar	•	KCL		0.8					SD Mesh	
Total flow basis	Mass	•		H2O (Populate PSD using	Populate PSD using				
Total flow rate		100 kg/hr	•	Total 1			O User-specified values					
							A distribution function					
							Distribution function					
							Туре	Normal	•			
							Standard deviation		1	cm	•	
							D50		2.4	cm	•	
										С	alculate	



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.

Ø Mixed	🕝 CI Solid	NC Solid	Flash (Options	EO Options	Costing	Comments]	
Specifi	cations								
Flash Type	Те	mperature	•	Pressur	re	Com			
State var	iables —			Mas	ss-Frac	-	Ŧ		
Tempera	ture		25	C	•		Component	t Value	e
Pressure			1	bar	•		KCL		
Vapor fra	action						AIR		1
Total flo	w basis	Mass	•			•	H2O		
Total flo	w rate		3000	kg/hr	-				
Solvent					~				
Reference	e Temperatu	ure							
Volume f	flow referend	ce temperature	e						
	C -								
Compon	ent concenti	ration referenc	e tempe						
	C						-		
					To	otal	1		

5.Click Next to go to Compressor Block.



🥝 Specifica	tions	Calcul	ation Options	Power	Loss	Converg	gence	Integration Parameters		
Model and Model	type — © Con	npresso	ri O	Turbine						
Type Isentropic										
Outlet spec	ificatio	n								
Oischarg	je pres	sure	6	bar		-				
Pressure	increa	se		bar		~				
Pressure	ratio									
🔘 Power re	quired			kW		Ŧ				
🔘 Use perf	orman	ce curve	es to determin	e dischar <u>o</u>	ge conc	litions				
Efficiencies										
Isentropic			Polytropic		Med	hanical				

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.

Specifications PSD Entrainment	Mass/Heat Transfer Atomization	🕝 Dry	ing Curve	Convergence	Utility	Comments
Operation mode	Continuous 🗸					
Dryer type:	Convective dryer 🔹					
Geometry						
Gas flow direction:	Cross-flow	•				
Solids flow:	Plug flow	•				
Input specifications:	Length	•	Solids res	idence time		•
Volume:			cum			*
Length:		4	meter			-
Cross sectional area:			sqm			Ψ
Solids residence time:		1.5	min			•
Solids velocity:			m/sec			*
Solids holdup:			kg			*
Fill grade:						
Bed porosity:		0.4				



Results

Summary	Balance	Evaporation	Profiles	ofiles Evaporation Ra		Utility Usage	Status
Exhaust gas	temperatur	e		276.304908	С		-
Calculated d	uty			1.4428e-08	Gca	l/hr	•
Solids reside	ence time			0.025	hr		•
Solids veloci	ty			0.0444444	m/s	ec	•
Critical mois	ture conten	ıt (dry)		0.0526316			
Equilibrium	moisture co	ontent (dry)		0.0309278	0.0309278		
Initial solids	moisture co	ontent (dry)		0.25			
Outlet solids	moisture c	ontent (dry)		0.0309278			
Overall evap	oration rate	e		17.5258	kg/ł	۱r	•
Initial inlet v	apor moist	ure content (dry))	0			
Outlet vapor	moisture c	ontent (dry)		0.00584192			
Vapor temp	at adiabati	c saturation		53.9143 C			•
Vapor moist	ure content	at adiabatic sat	uration	0.109343	0.109343		
Calculated L	ewis numbe	er		0.805167			
Calculated h	eat transfer	coefficient		1502.07	kcal,	/hr-sqm-K	•

N	laterial	Heat	Load	Vol.% Curves	Wt. %	Curves	Petroleum	Polymers	Solid	s		
							Units	CA	•	SI 🔹	AO •	so •
	Ν	lass Der	sity			kg/cum	1	3.6	5269	1656.38	0.631502	1835.84
	E	Enthalpy Flow				Gcal/hr		0.1	9935	-0.187651	0.128439	-0.116741
	А	Average MW						28.9509		45.8031	28.8492	68.1362
	+ N	+ Mole Flows				kmol/h	nr	103	3.624	2.18326	104.597	1.21043
	+ N	/lole Fra	ctions									
	- N	lass Flo	ws			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
	+ N	+ Mass Fractions										
	v	Volume Flow				cum/hr		82	1.313	0.0603725	4778.33	0.0449245



Example: KCL CRYSTALLIZATION

Consider the process of KCI crystallization from KCI 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 KCI 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.

Selection Petroleum	n Nonconventional	Enterprise Database	Comments				
elect components							
Component ID	Тур	e	Component na	me	Alias	CAS numbe	
KCL(S)	Solid		POTASSIUM-CHLORID	E KCL		7447-40-7	
H20	Conventional		WATER	H2C)	7732-18-5	
KCL	Conventional		POTASSIUM-CHLORID	E KCL		7447-40-7	
*							
Find Elec Wiz	ard SFE Assistant	User Defined	Reorder	w			
_		Y					
Global Flo	wsheet Sections	Referenced	Comments				
- Property metho	ds & options —		Method name				
Method filter	Соммо	N -					
Base method	SOLIDS	-	SOLIDS	•	Metho	ds Assistant	
Henry compone	ants	•	C Modify				
Themy compone	51105		Vapor FOS	F	SIG	-	
Petroleum cal	culation options		Data act		.510		
Free-water me	ethod STEAM-T	A -	Data set				
Water solubili	ty <u>3</u>	-	Liquid gamr	na	IDL	*	
			Data set			1 🚔	
Electrolyte ca	Iculation options	5	Liquid mola	r enthalpy 📕	ILMX108	*	
Chemistry ID		•	Liquid mola	r volume 🛛 🛛	LMX25	*	
🚺 Use true co	omponents		Heat of	mixina			
			Dounting	correction			
			Poynting correction				

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).

🥑 Mixed	🥝 CI Solid	NC Solid	Flash (Options	EO Options	Costing	g Comments		
Specific	ations								
Flash Type	Ten	perature	•	Pressur	e	Cor	nposition —		
State varia	ables					M	ass-Frac	•	~
Temperat	ure		25	с	-		Component	: Val	ue
Pressure	Pressure			bar	-		KCL(S)		
Vapor frac	ction						H2O		0.74
Total flow	/ basis	Mass	-			•	KCL		0.26
Total flow	/ rate		1000	kg/hr	-				
Solvent					-				
Reference	e Temperatur	e				_			
Volume fl	ow reference	e temperature	e						
	C -								
Compone	ent concentra	tion reference	e tempe	erature					
	C T								
							Tc	otal	1



Under "Solids" folder, selectwater as the moisture component, as shown in Figure 14.27.

Solid Charact	terization 🛛 🔗 PSI	D Mesh Substreams	
Stream class	MIXCIPSD •	Moisture components - Available KCL	Selected

\bigcap	Mesh Commer	nts					
F	SD mesh ID	PSD		- Part	icle size distribut	tion mesh ——	
	DSD Mash				Int.	Lower	Upper
					1	0	0.5
	PSD mesh type	Equidistant			2	0.5	1
	No. of intervals	10 🚭			3	1	1.5
	Lower limit	Upper limit	Size units		4	1.5	2
	0	5	cm 👻		5	2	2.5
					6	2.5	3
			Create PSD Mesh		7	3	3.5
	Cautions If you are				8	3.5	4
	lost for the remov	uce the number of i ved intervals whereve	ntervais, data will be ar this PSD is used		9	4	4.5
					10	4.5	5

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 KCI 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) \rightarrow KCl(S).

Specifications	🔮 Crystallizat	ion 🛛 🥑 Sol	lubility	Recirculation	⊘ PSD	Crystal Growth	Flash O	ptions	Comments
Operating condition	ons ———								
Pressure		•		*		1 bar	-		
Heat duty		-		~	30	00 kW	•		
Coturation colculat	tion mothed	Calt aposifi	cations					J	
 Saturation calculation Solubility data 	tion method	Salt compo	cations -		~				
Solubility funct	ion	Move o	rvstallizir	ng salt from CL	Solids substr	eam			
Chemistry			rvetalliza	d salt to CI Soli	de substrean	n			
User subroutine	e	Move c	rystamze		us substream				
]							ļ	
Valid phases			perating	mode					
Vapor-Liquid		- (Crystallizi	ing		•			

Specifications	Crystallization	🥝 Solubility	Recirculation	🔮 PSD	Crystal Growth	Flash Options	Comments
Specifications Reactants Component KCL	Coefficient -1	Crystal KCL(S Coeffic	Recirculation product (CIPSD) ient 1	♥ PSD	Crystal Growth	Flash Options	Comments
Stoichiometry — KCL> KCL(S) (C	:IPSD)						



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.

ſ	Specifications	Crystallization	Solubility 🎯	Recircul	ation	🕜 PSD	Crystal Growth	Flash Options	Comments
	Solubility basis — Solvent	H20	•						
	Solution								
	Solubility data								
	Solubility data type	Ratio		•	Temp	erature	Ratio		
					С	•			
				•		25	0.35		
L									

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.

Specifications Crystallizatio	on Solubility	Recirculation	🥑 PSD	Crystal Growth	Flash Optio	ns Comments
PSD calculation option Copy PSD from inlet Calculate PSD from growth kinet Calculate PSD from particle grow User-specified PSD Overall Substream ID	tics wth model	rstallizer volume – 4 cu	m	•		
User-specified PSD Use distribution function User-specified PSD						
Bypass fraction: Distribution function ID	0 🔇 1 🗸					
Distribution function: Select parameters:	Normal D50	•	· Standa	rd deviation	•	
D50:	2	cm -	·			



Results

Summary	Balance	Pro	ofiles	PSD	Results	▲ Status		
Constallizar t	mooratura				01 027	<u>с</u>		
Crystallizer to	emperature				101.957	· ·		
Heater duty					300	kW 🔻		
Net duty					0	Gcal/hr 🔹		
Crystallizer p	ressure				1	bar 🔹		
Crystallizer v	olume				4	cum 🗸		
Residence tir	me			7	7.80996	hr 🔹		
Crystal produ	uct		133.127			kg/hr 🔹		
Vapor flow r	ate			3	377.506	kg/hr 🔹		
Recirculation	n flow rate		0			kg/hr 🔹		
Magma dens	259.928			gm/l 🔹				

Material	Heat	Load	Vol.% Curves	Wt. %	Curves	Petroleum	Polymers	Solid	5	
						Units	FEED	•	PRODUCT •	VAPOR -
	Temperate	ure			С			25	101.937	101.937
•	Pressure				bar			1	1	1
	Molar Vapor Fraction							0	0	1
	Molar Liqu	uid Fract	tion					1	0.924363	0
	Molar Soli	id Fracti	on					0	0.0756368	0
	Mass Vapo	or Fracti	on					0	0	1
•	Mass Liqu	id Fracti	on					1	0.78614	0
	Mass Solid	d Fractic	n					0	0.21386	0
•	Molar Ent	halpy			kcal/m	ol	-70).7673	-71.9398	-57.1363
•	Mass Enth	alpy			kcal/kg		-31	153.66	-2728.42	-3171.55
•	Molar Ent	ropy			cal/mo	I-K	-37	7.5682	-32.1967	-8.73304
	Mass Entro	ору			cal/gm	-К	-1.	67418	-1.22111	-0.484757
	Molar Density				mol/cc		0.05	09796	0.0460964	3.20657e-05
•	Mass Den	sity			kg/cum	1	1	143.97	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		
НуСус	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.1Solids Classification Based on Knowledge of Molecular Structure and Chemical Reactivity.					
Class	Туре	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

	00	Selection	Petroleum	✓ Nonconventional	Enterprise Databas	e Comments			
S	Select components								
	Component ID		ent ID	Туре		Component name		Alias	CAS number
	WATER Conventional			WATER		H2O	7732-18-5		
	NACL Solid		SODIUM-CHLORIDE		NACL	7647-14-5			
	Þ	NA+ Conventional		NA+		NA+			
		CL-	Co	Conventional		CL-		CL-	
		PTA Conventional			TEREPHTHALIC-	ACID	C8H6O4-D3	100-21-0	
	Þ	PTA(S) Conventional		TEREPHTHALIC-ACID		C8H6O4-D3	100-21-0		
	Þ	COAL	Nonconventional						
		SIO2	Solid		SILICON-DIOXID	E	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.

Mixers/Splitters Sep	rators Exchangers	Columns Reac	ctors Pressure Changers	Manipulators	Solids Solids Separators	Batch Models User Models
MULT UDUPL Mult Dupl	CIChng	Analyzer	lector	tHARGEBAL Chargebal Measure	ement Design-Spec	ALCULATOR TRANSFER TRANSFER Transfer

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:



TABL	TABLE 14.D.1Substream Classes for Solid-Bearing Streams.				
#	Substream Class	Description			
1 2	MIXED CISOLID	Fluids only Conventional inert solids that participate in reactions but do not participate in phase equilibria (except in the RGibbs model)			
3 4 5	NC NCPSD CIPSD	Non-conventional solids Non-conventional solids with PSD 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

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.



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





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.

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