Optimization of Fluidized Bed Reactor Using Aspen Plus

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Abstract:

Fluidized bed reactor is useful for heterogeneous (multiphase) reactions, separations, size enlargement, coating, and blending in chemical and pharmaceuticals industries. To develop a model and simulation of this reactor with advanced systems process engineering software (Aspen Plus). Aspen plus has the capability to simulate real factory performance, design improved plants, and intensify profitability in present plants. This modeling and simulation are applied Geld art B particle classification, GGC is used for particle size distribution function, Newton parameters for mass convergence, and Ergun equation is used for minimum fluidization velocity calculation and pressure drop through the fluidized bed reactor. Generally, most of the predictions model from Aspen plus is a reasonable agreement through the experimental results. Advantage of this investigation is used small quantity of bed particles and identified their melting point temperature is above 340°C. This fluidized bed reactor model and simulation is functional for aluminum hydroxide decomposition reaction. The feed 275 kg/hr of Al(OH)3is converted into 169.6 kg/hr of aluminum oxide (Al2O3) and 89.9 kg/hr of water. A total mass conversion percent is 94.4% of aluminum hydroxide.

Introduction:

Introduction to Aspen Plus modeling and simulation of Al(OH)3 decomposition reaction: The decomposition of aluminum hydroxide into aluminum oxide and water within a fluidized bed reactor serves as the focal point of this study. The resulting product, alumina (aluminum oxide), finds extensive utility across various sectors, including adsorbents, catalysts, microelectronics, chemicals, aerospace, and high-technology fields. Previous literature has emphasized the diverse applications of alumina, highlighting its role as an inert biomaterial and a material compatible with biological environments, alongside its significance in aluminum metal production and abrasives due to its exceptional hardness and high melting point. The chemical reaction mechanism governing this process is represented by the stoichiometric equation:

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

Indicating the conversion of two moles of aluminum hydroxide into one mole of alumina and three moles of water. The rate of this reaction is expressed through first derivative equations, elucidating the kinetics involved in the transformation.

The fluidized bed reactor stands as a versatile unit operation within the chemical and pharmaceutical industries. Its functionalities encompass a wide range of operations, including biomass steam gasification, hydrocarbon cracking to produce lighter molecules, and the coating and blending of pharmaceutical products. In our current study, we utilize a fluidized bed reactor for the decomposition of aluminum hydroxide. Employing advanced system process engineering software such as Aspen Plus allows for modeling and simulation to achieve maximum yield of alumina (Al2O3) while minimizing the use of solid bed particles. Aspen Plus, recognized as a pivotal tool in computer-aided process engineering, is endorsed by CAPE-Open, a platform for open access in this field.

This chemical process simulation software, exerts significant influence on the design and operation of chemical engineering products. Its capabilities extend to optimizing processing conditions, reducing experimental time, and conserving energy. Aspen Plus, renowned for its accuracy in modeling thermodynamic properties and facilitating the separation of real mixtures, boasts extensive databases for generating parameters. Catering to a diverse array of industries including synthetic substances, polymers, specialty chemicals, metals and minerals, and coal power, Aspen

Plus serves as a commercial software tool for designing, optimizing, and monitoring processes. Notably, it excels in handling complex operations such as multiple-column separation systems, reactors, heat exchangers, and pressure changers, contributing significantly to enhanced efficiency and productivity in industrial settings.

In this project, Aspen plus software is the main tool and method for modeling and simulation an aluminum hydroxide decomposition reaction. To predict the fluidized bed reactor geometry, processes variables, reaction kinetics parameters, conversion of desired product, and operable operations conditions.

Aspen Plus Setup for Fluidized Bed Reactor:

Setting up Aspen Plus for a fluidized bed reactor is a crucial step in accurately modeling and simulating the reactor's behavior. Aspen Plus offers a comprehensive platform for process simulation, allowing engineers to design and optimize various chemical processes. The fluidized bed reactor, with its widespread applications in industries such as chemical and pharmaceutical, presents unique challenges in terms of modeling its complex behavior. Therefore, a systematic approach is necessary to ensure that Aspen Plus accurately represents the fluidized bed reactor's dynamics and performance.

Setting up Aspen Plus for a fluidized bed reactor involves several key steps. First, engineers must define the components and reactions involved in the reactor system. This includes specifying the reactants, products, and any intermediates, as well as the chemical reactions that occur within the reactor. Careful consideration must be given to the kinetics and stoichiometry of these reactions to accurately model their behavior. Once the components and reactions are defined, engineers must select appropriate thermodynamic models for the system. Aspen Plus offers a wide range of thermodynamic models, allowing users to choose the ones that best represent the behavior of their specific system. These models will play a crucial role in determining the thermodynamic properties of the components and reactions within the fluidized bed reactor.

With the components, reactions, and thermodynamic models defined, engineers can then proceed to create the fluidized bed reactor within the Aspen Plus environment. This involves specifying the reactor type (e.g., fluidized bed), dimensions, operating conditions, and any other relevant parameters. It is essential to accurately represent the geometry and behavior of the reactor to obtain reliable simulation results. Once the reactor is set up, engineers must specify the operating conditions, including temperature, pressure, flow rates, and residence time. These parameters will influence the behavior of the reactor and the conversion of reactants to products. Engineers should also consider heat and mass transfer phenomena within the reactor, specifying relevant parameters such as heat transfer coefficients and mass transfer coefficients. After configuring the reactor and specifying the operating conditions, engineers can run the simulation in Aspen Plus. During the simulation, they should monitor for convergence and stability, adjusting solver options as needed to ensure accurate results. Finally, engineers can analyze the simulation results to gain insights into the performance of the fluidized bed reactor, evaluating key metrics such as conversion efficiency, product yields, and energy consumption.

Thermodynamics physical properties method for Sample preparation:

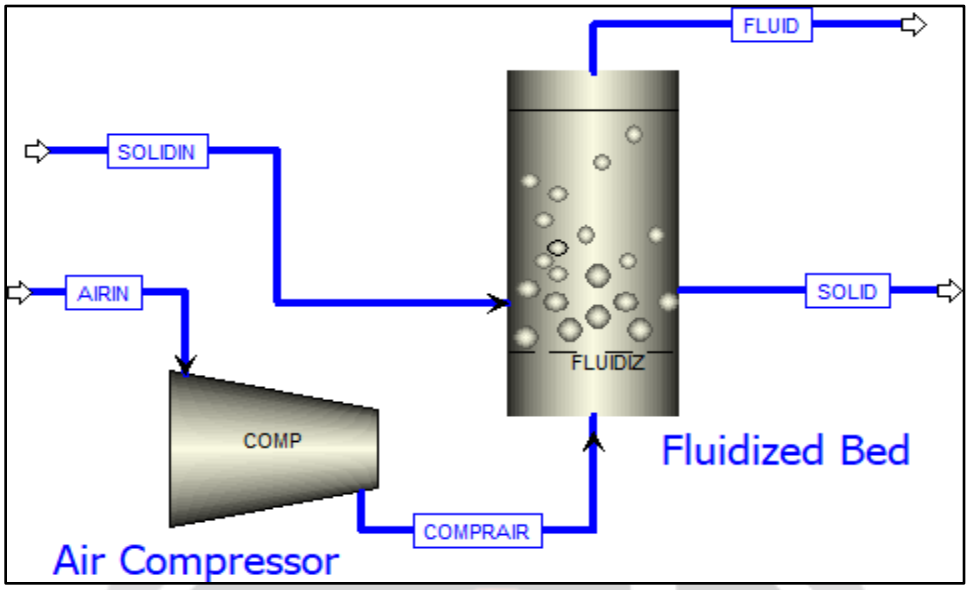
When opening the Aspen Plus template, choose a solid with metric solids. This choice helps set boundary conditions during the simulation process. Next, specify the components by their IDs, types, names, and aliases. Gas and liquid components fall under a category called conventional, while solid components are categorized as solid. In this particular process, four main components are involved. as table-1 below show components specifications,

Once the component specifications are complete, the next step is to choose the best methods based on the behavior of each component in the production process. This involves considering the physical properties of the components and selecting appropriate methods for modeling and simulation. For instance, in the case of the aluminum oxide production process, a table (Table-2) summarizes the specifications of methods to be used.

Methods Specifications			
Method filter is selected	ALL	method name is selected	SOLIDS
Base method is selected	SOLIDS		
Petroleum calculation options			
Free water method is selected	STEAMNBS		
Water solubility is selected	3		

In Aspen Plus simulation, the graphical user interface (GUI) is referred to as the main flow sheet. Within the main flow sheet window, various unit operations and materials are organized in folders within the model palette, typically located at the bottom or sometimes at the top right of the interface. Figure 1 depicts the process flow sheet for the production of aluminum oxide. This visual representation showcases the sequence of operations and materials involved in the production process.

Component ID	**Type**	**Component name**	**Alias**
Alumi-01	Solid	Aluminum-Hydroxide-Amorphous	Al (OH)3-A
Alumi-02	Solid	Aluminum-Oxide-Alpha-Corundum	Al2O3
Air	Conventional	Air	Air
Water	Conventional	Water	H2O



Descriptions of Aspen plus Simulation Setup:

Setting up a simulation in Aspen Plus involves a series of steps to accurately model chemical processes. Initially, you define the chemical components present in your system and specify their properties, such as molecular weight and critical properties, along with choosing appropriate property methods for thermodynamic calculations. Then, you construct the process flowsheet within the main flow sheet window by selecting and arranging unit operations from the model palette. Each unit operation represents a stage in your process, such as reactors, separators, or distillation columns, and you connect them to define material flow. Next, you specify the inlet and outlet conditions for each stream, including flow rates, compositions, temperatures, and pressures. After configuring unit operation models with the appropriate parameters and operating conditions, you set up any necessary recycles and process specifications to achieve desired process performance. Aspen Plus performs thermodynamic and physical property calculations based on the specified components, property methods, and stream conditions, crucial for predicting phase equilibria, chemical reactions, and heat transfer. Running the simulation iteratively solves material and energy balances throughout the process to obtain a steady-state solution. Finally, you analyze the results using Aspen Plus tools, such as stream tables and customizable reports, to understand process behavior, optimize design, and improve operational efficiency through iteration and optimization. Overall, Aspen Plus facilitates the comprehensive modeling and analysis of complex chemical processes, aiding in the development and refinement of industrial processes across various sectors.

Streams inlets:

Stream name: Air in (into Air Compressor)				
State variables	**Amounts**	**Units**	**Composition in mass fraction**	
Temperature	25	°C	**Components**	**Value**
Pressure	1	bar	Al (OH)3	
Total flow basis	mass		Al_2O_3	
Total flow rate	4150	kg/hr	H_2O	
			Air	1
Stream name: Solid in (into Fluidized)				
State variables	**CIPSD**	**units**	**Composition in mass fraction**	

Temperature	25	°C	**Components**	**Value**
Pressure	11	bar	$Al(OH)_3$	1
Total flow basis	mass		Al_2O_3	
Total flow rate	275	kg/hr		

Operations Conditions of Air Compressor:
An air compressor makes the air stronger by increasing its pressure. This pressurized air can then easily move through the material in a bed. There's a specific type called Isentropic compressor. If we want to make sure it works well, we check that it can produce air at a pressure of 11 bar at the outlet.

Operations Conditions of Fluidized bed:
When using simulation software like Aspen Plus to model fluidized beds, you need to specify various operating conditions. This includes details like the amount of material in the bed, the shape and size of the column, how the gas is distributed, any chemical reactions happening, and ensuring the simulation runs smoothly, which is called convergence.

Stoichiometry specifications			
Rxn No.	Reaction type	Stoichiometry	
1	Kinetic	2 $Al(OH)_3$(CIPSD)	Al_2O_3 (CIPSD) + 3 H_2O
Kinetic specifications			

Reacting phase =>Vapor		Rate Basis =>Reac (Vol)
Pre-exponent K_0 value	0.39	
Activation Energy	7253.84	cal/mol

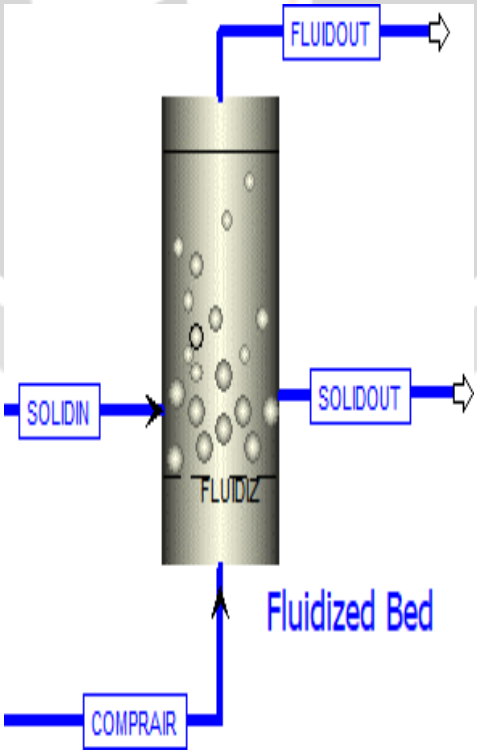
A pre-exponent rate of constant and activation energy was taken from experimental published work by American Institute Chemical Engineers journal as book chapter (Candela 1986).

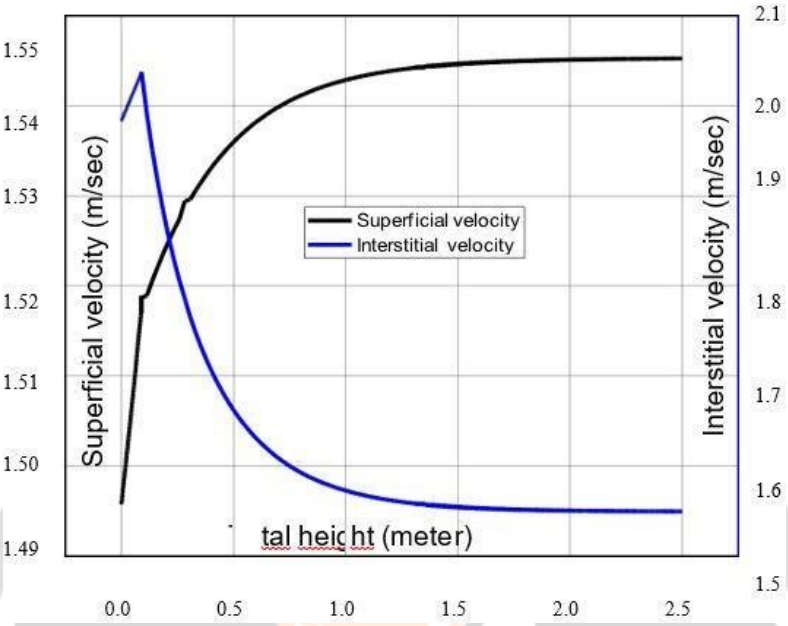
Specification				**Geometry of Column**		
parameters	value	units		parameter	value	unit
bed mass	50	kg		Height	2.5	m
voidage @min fluidization	0.5			Solid outlet	0.75	m
Geld art classification	Geld art B			Diameter	0.4	m
min. fluidization velocity	Ergun equations			**Gas Distributor**		
TDH model	George & Grace			type	perforated plate	
max. dC/dh	1.00E-05			number of orifices	40	
Elutriation model	Tasirin & Geldart			orifice diameter	10	mm

Results and Discussions:
After running the simulation, we get a summary table called "Stream Result" which shows all the details of what's going into and coming out of the process. In this specific case, let's say we're decomposing aluminum hydroxide. We

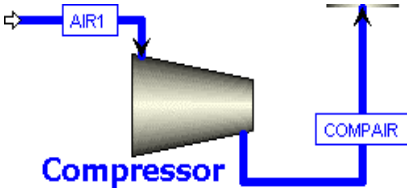
start with 275kg/hr of aluminum hydroxide going into a fluidized bed reactor. To remove the water molecules from the aluminum hydroxide, we use compressed air at a rate of 4150kg/hr, at a high pressure of 11 bar (which corresponds to a temperature of 422.8°C). According to the decomposition reaction $2Al(OH)3 \rightarrow Al2O3+3H2O$, after the reaction takes place, we find that 169.6kg/hr of aluminum oxide and 89.9kg/hr of water are formed. This leaves 15.42kg/hr of aluminum hydroxide remaining. All these details, including input and output quantities, are listed in a table called "Stream Result" for easy reference and analysis. It's like a snapshot of what's happening in the process.

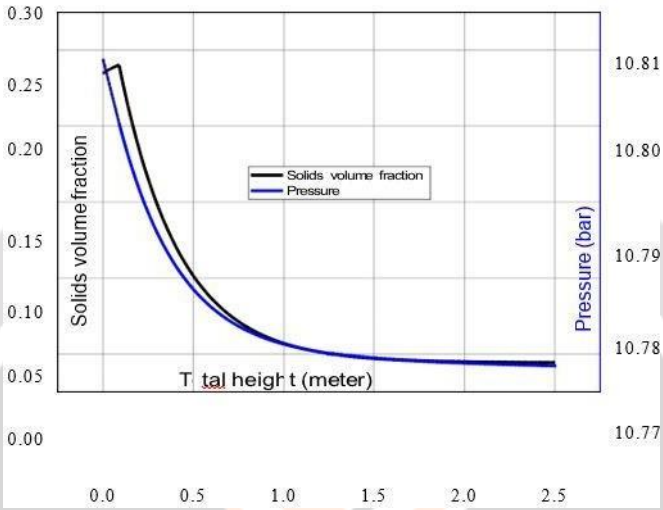
Process variables	Air in	Comp Air	Solid in	Fluid out	Solid out
Temperature °C	25.0	422.8	25.0	338.8	338.8
Pressure bar	1.0	11.0	11.0	10.8	10.8
Mass VFrac	1.0	1.0	-	1.0	-
Mass SFrac	-	-	1.0	< 0.001	1.0
All Phases					
Mass Flow kg/hr	4,150.0	4,150.0	275.0	4,240.9	184.1
Volume Flow cum/hr	3,553.4	754.1	0.1	700.9	0.0
Enthalpy Gcal/hr	< 0.001	0.4	-1.1	0.0	-0.7
Density kg/cum	1.2	5.5	2,600.1	6.1	3,812.8
Mass Flow kg/hr					
Aluminum hydroxide			275.0	0.1	15.4
Alumina				0.9	168.7
Water				89.9	
Air	4,150.0	4,150.0		4,150.0	





Parameters and Process variables	Value
Height of bottom zone [meter]	0.089511457
Height of freeboard [meter]	2.41048854
TDH from correlation [meter]	2.23125858
TDH based on solids volume profile [meter]	2.41048854
Solids holdup [kg]	50.0001362
Number of particles in bed	5970160.15
Bed surface area [sqm]	20.2918358
Distributor pressure drop [bar]	0.19113425
Bottom zone pressure drops [bar]	0.008463783
Freeboard pressure drop [bar]	0.031979177
Fluidized bed pressure drops [bar]	0.04044296
Overall pressure drops [bar]	0.23157721
Heat duty [Gcal/hr]	0
Minimum fluidization velocity [m/sec]	0.724609882
Heat exchanger duty	
Bed temperature [°C]	338.845523
Moles generated from reaction [kmol/hr]	3.32676322





Compressor model	Isentropic Compressor
Phase calculations	Vapor phase calculation
Indicated horsepower [kW]	471.467579
Brake horsepower [kW]	471.467579
Net work required [kW]	471.467579
Power loss [kW]	0
Efficiency	0.72
Mechanical efficiency	1
Outlet pressure [bar]	11
Outlet temperature [C]	422.81062
Isentropic outlet temperature[C]	314.422948
Vapor fraction	1

After completing the modeling and simulation, we've got a graph called "Figure-4" that shows two important things about the fluidized bed column.

First, there's a black line on the graph. This line represents the distribution of solid particles throughout the height of the column. At the bottom of the column, the particles are packed tightly, and as you move upwards, their density decreases exponentially until it reaches zero at a height of 1.5 meters. This means that there are no particles or catalysts left in the outlet of the column. Based on this, it's recommended that the total height of the column should not exceed 2.5 meters.

Second, there's a blue line on the graph representing the pressure drop throughout the column. This pressure drop also decreases exponentially as you move through the column. This drop happens because of the presence of bed particles and solid materials. Essentially, it shows how the pressure changes as the fluid moves through the column filled with particles.

Conclusion:

The Aspen Plus software was used to model and simulate a fluidized bed reactor for decomposing aluminum hydroxide. The model used parameters like particle size distribution and Newton's method for convergence. It predicted that the best temperature for the bed particles (catalyst) should be above 340°C to prevent them from melting. The simulation showed that the reactor could convert 94.4% of the aluminum hydroxide into aluminum oxide and water. The feed rate was 275 kg/hr of aluminum hydroxide, which resulted in 169.6 kg/hr of aluminum oxide and 89.9 kg/hr of water. Overall, the model suggested good efficiency for this reaction.

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