

## Use Advanced Simulation to Improve Processes Involving Solids

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## Executive Summary

This paper describes the approach in Aspen Plus® for incorporating granular solids and the corresponding solids processing steps when modeling processes. Modeling the solids section of a process is important for many common processes including specialty chemicals, agrochemicals, metals and mining, pharmaceuticals, biofuels and more. The main challenges that arise when optimizing or troubleshooting a solids process include inefficient designs due to separate modeling of fluids and solids sections, overdesign of equipment, high-energy demands, reduced yields and quality variability.

As contrasted to fluids, which are generally described by concentrated properties like vapor fraction, composition, temperature and pressure, granular solids are described by distributed properties such as particle size distribution (PSD). This adds an extra level of complexity to the description of the material, and therefore the solids section of a process is often neglected or oversimplified.

Whether particles are being formed (e.g., crystallization, spray drying), reduced in size (e.g., crushing/grinding), enlarged (e.g., granulation, agglomeration), participating in reactions (e.g., fluidized bed reactor, fixed bed reactor) or just being separated from a fluid stream (e.g. cyclones, filters, centrifuges), ignoring or poorly modeling the solids processing steps may lead to lost opportunities, including costs reductions and quality improvements. Considering this, some companies use in-house models or spreadsheets to describe the solids section of a process.

## Process engineers who are not solids modeling experts can use conceptual models to develop an initial design.

The drawback of this custom or “one-off” approach is that the fluid section of the process is modeled in one simulation environment (such as Aspen Plus), while the solids section is modeled in another (like Excel). In general, this approach may lead to errors and inefficiencies due to data transfer, different stream structures or inconsistent physical properties.

Aspen Plus process simulation software provides the capability to describe granular solids in detail and provides a comprehensive model library for the equipment associated with solids processing steps. The model library covers drying, fluidization — including chemical reactions, granulation, crystallization, crushing and grinding — classification, solid/liquid and gas/solid separation, as well as pneumatic conveying of solids. The Aspen Plus user can consequently model processes that contain both fluids and solids in one simulation environment using consistent physical properties to avoid errors and inefficiencies that may result from the transfer of data from one simulation system to the other.

The unit models offered in the library can range in fidelity from conceptual to rigorous. Process engineers who are not solids modeling experts can use conceptual models to develop an initial design before handing it off to a solids expert for more rigorous design, if needed. Activated features in Aspen Plus such as Economics, Energy and Exchanger Design and Rating are available to further optimize processes that contain solids sections.

Over 450 organizations currently use AspenTech’s innovative solids modeling, and their feedback has been very positive.

# Introduction

In addition to fluids, many industrial processes involve solids processing steps that often have a significant influence on the overall process performance, product quality or energy demand. In general, the solids section of an industrial process has to fulfill one or more of the following tasks:

- Formulate particles (e.g. granulation, crystallization, spray drying)
- Adjust the moisture content (e.g., drying)
- Change the composition by chemical reactions (e.g., fluidized bed reactor)
- Adjust the particle size distribution (crushing/grinding, classifying, compacting)
- Separate solids from a fluid (e.g., cyclone, centrifuge)

In designing, revamping or troubleshooting a process with a solids section, four main interconnected challenges typically arise:

- **Separate Design of Fluid and Solid Sections of a Process**
  - The influence of the solids section on the overall process performance is very often either neglected, described by use of very simple splitter models or by use of spreadsheet tools or in-house codes. The fluid part of a process is typically modeled in a process simulator, while particle scientist within the same company model the solids part of the process in another tool.
  - This approach may lead to errors and inefficiencies due to data transfer, different stream structures or inconsistent physical properties. Furthermore, recycle streams from the solids section to the fluid section upstream in the process could only be considered in a very limited way. An additional limitation is that the optimization of the overall process is more or less impossible by use of this workflow.



- **High Capital Costs Due to Overdesigned Equipment**

- To reduce the risk of bottlenecks, equipment is often designed in excess leading to exaggerated capital costs. Rigorous modeling can allow for more appropriately sized solids processing equipment and reduce recycle streams to minimize the load of equipment. Examples of solids processing equipment that is often overdesigned are crushers, compactors and dryers.
- In most cases, one or several recycles are used to reprocess too coarse or too fine particles. Reducing these recycle streams can help eliminate bottlenecks that limit product throughput and is key to reducing the loadings on certain crushers and compactors, allowing for smaller, less expensive equipment.

- **High Operating Costs Due to Excess Energy Demands**

- For many applications, intermediate or final products need to fulfill very tight specifications regarding their moisture content to be used for subsequent process steps or to be sold as final products. In some cases, liquid and solid separation is used for the initial dewatering of solids to remove excess water.
- After dewatering, the removal of the remaining moisture content is completed using drying. Similarly, particles that are formulated, for example, by a crystallization step or are entrained from a fluidized bed with the gas stream may need to be separated from the surrounding fluid and be recycled back to the main solids stream in the process. The separation of solids and gas involves gas cyclones, scrubbers, fabric filters or electrostatic precipitators.
- To ensure that particles are dried to contain adequately low moisture and that the maximum amount of solid products or intermediates is separated by liquid streams, excess energy may be used. By modeling these steps both rigorously and in larger processes, substantial energy savings may be unlocked (up to 30 percent has been seen in the case of drying).



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- **Reduced Throughput and Quality of the Product**

- The design of a profitable process hinges on the throughput and the quality of the final product. While it is important to produce a large quantity of products to offset operating costs, it is also important to maintain the quality of a product to appease customers. The selectivity of reactions and the formulation of particles are examples of where both quality and quantity can be improved.
- For many important industrial processes, solids can act as educts or a catalyst in chemical reactions and therefore have a major influence on the selectivity and the yield of the reactor. Starting from a solution or slurry, particles are formulated with the aim to produce a dust free, free flowing powder with well-defined properties. This is done in most cases by crystallization, granulation/agglomeration or spray drying. The design and operating conditions of these units can determine the PSD and moisture content of the product.
- Similarly, avoiding downtime that may result from unnecessary maintenance, such as clogged solids handling systems, can improve throughput. Conveying is used to transport solids through pipes and understanding the pressure drops and velocities needed to avoid clogging while still reducing energy costs is important for increasing uptime and, therefore, throughput.

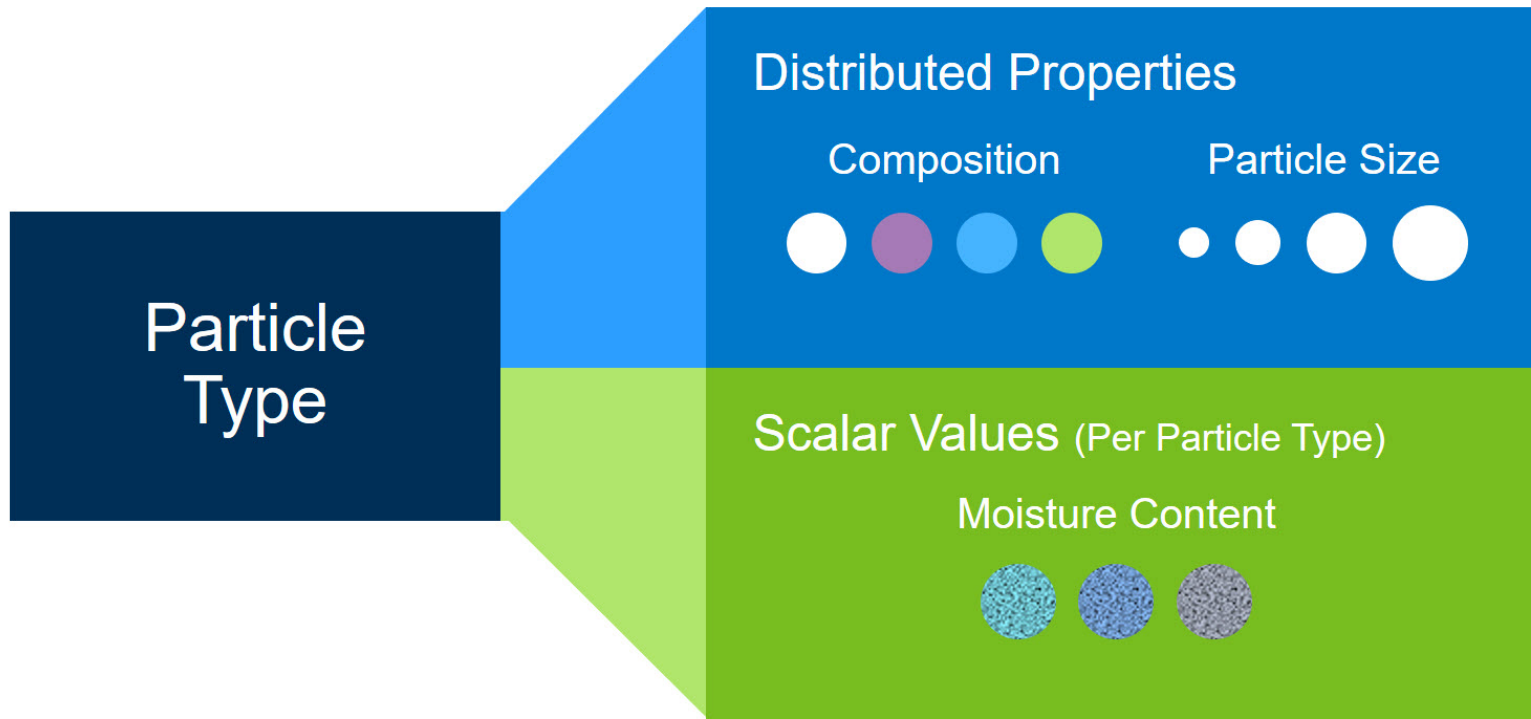


Figure 1: Schematic of the solids characterization in Aspen Plus

## Implementation of Solids Modeling in Aspen Plus

### Particle Characterization: The Key to Understanding Solids Processing

In Aspen Plus, dispersed solids can be characterized in detail (as schematically shown in Figure 1). Users can define multiple particle types, with different distributed properties such as composition and particle size. In addition, it is also possible to define the moisture content of the particles as a loading of one or more fluid components.

The defined moisture content has an influence on the particle's heat capacity and density, thus having an impact on its settling velocity. As a result, wet particles will be separated differently in a classifier than dry particles with the same particle size distribution (PSD).

Additionally, an intuitive and easy-to-use workflow for the definition of particle size distributions has been integrated in to Aspen Plus. It consists of the following steps:

- **Definition of the particle size classes (particle size mesh)**  
Aspen Plus offers an automated and a manual mode to generate the particle size classes that should be used to describe the PSD. The user can select a predefined mesh type (e.g., equidistant, geometric or logarithmic) in automated mode or the user can import measured data from a particle size analysis in manual mode.
- **Definition of the mass fraction within the different particle size classes**  
For the definition of the mass fractions, Aspen Plus offers an automated or manual mode. In the automated mode, the user can define mass fractions by selecting a distribution function (e.g., GGS, RRSB [Rosin Rammler Sperling Bennet], log-normal or normal distribution) and enter a value for the shape (e.g., dispersion parameter) and the position parameter (e.g., characteristic diameter  $d_{63}$  or  $d_{50}$ ). In the manual mode, the user defines the mass fractions as tabular data, such as from measured data found during a particle size analysis.

By opening the stream results, users can visualize the defined and calculated particle size distributions with a click of a button in form of a cumulative mass, density or RRSB distribution. It is also possible to show the PSD for different particle types and streams in the same plot and compare inlet and outlet streams of a unit operation to fully understand how certain unit operations change the particle size distribution of feed material. An example of how a double-deck screen changes the PSD is shown in Figure 2.

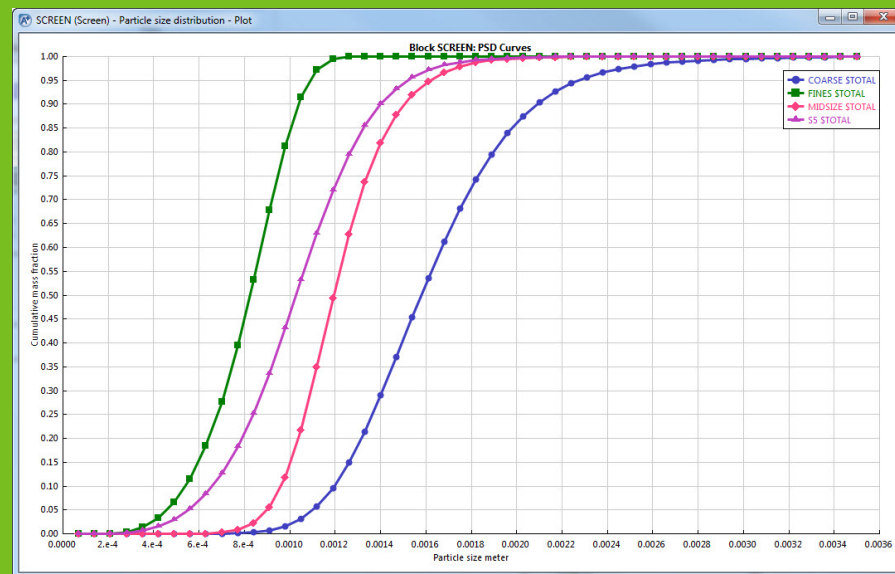


Figure 2: Cumulative particle size distributions for the stream entering (purple) and the three streams leaving (fines: green, midsize: pink, coarse: blue) the screen



In addition to the plot of the particle size distribution of the streams, the user can easily generate plots that are specific to a unit operation. This could be the solids volume concentration profile of a fluidized bed or the solids temperature and moisture profile in a convective dryer. As an example, Figure 3 shows the separation efficiency curve of the double-deck screen used in the example above.

### Solids Modeling Unit Library

The solids modeling library in Aspen Plus contains 17 solids blocks (as shown in Figure 4). The design philosophy used here is that one block can represent many different types of equipment at different levels of fidelity from conceptual to rigorous. In total, the solids model library contains over 80 different equipment models.

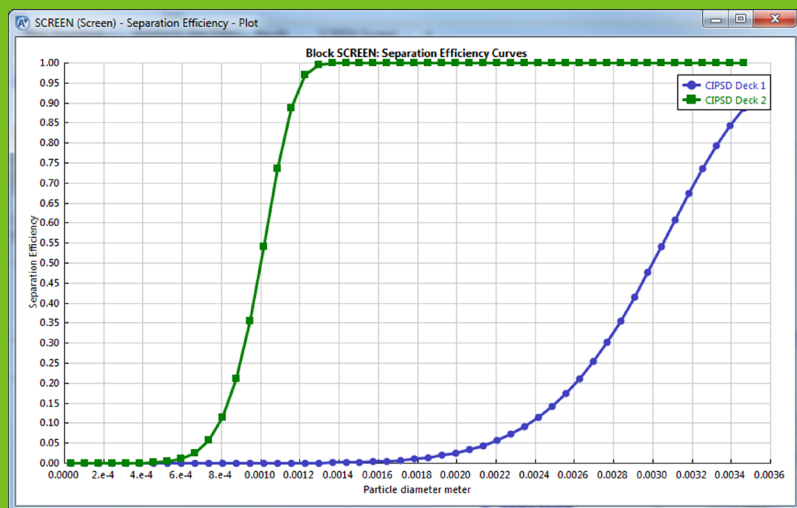


Figure 3: Example separation curves for a two-deck screen

Formulate Particles	Adjust Moisture	Chemical Reactions	Adjust PSD	Solids & Liquids Separation		Solids & Gases Separation	Transport Solids
 Crystallizer	 Convective Dryer	 Fluidized Bed Reactor	 Crusher / Mill	 Hydro Cyclone	 Centrifuge	 Gas Cyclone	 Single Pipe
 Granulator/Agglomerator	 Contact Dryer	 CSTR, Rbatch, RPlug	 Classifier	 Cross Flow Filter	 Liquid Filter	 Scrubber	 Pipe Network
 Spray Dryer			 Screen	 CCD	 SWash	 ESP and Fabric Filter	

Figure 4: Solids modeling unit operations in Aspen Plus



- **Crystallization:** Simulate continuous and batch crystallizers using a rate-limited nucleation/growth model and account for reactions, spontaneous nucleation and seed crystallization.
- **Granulation:** Use the granulation model to describe fluidized bed spray and high-shear granulation and agglomeration.
- **Spray Drying:** Model a wide range of industrial spray dryers for pigments, catalyst product, etc.
- **Drying:** Use rigorous and conceptual methods to model contact dryers, fluidized bed dryers, belt dryers, flash dryers and more. In the contact dryer, options include an inlet gas stream, co-current flow, heat transfer from wall to solid phase and gas and solid phase.
- **Fluidized Bed:** Consider chemical reactions and their impact on fluid mechanics. Get a better understanding of re-circulation rates and particle size distributions throughout the production process. Minimize loss of fines and recycle rates, and improve yields and selectivity.
- **Crushing, Milling:** Prevent oversized equipment with high-fidelity models of grinding and crushing. Simulate wet and dry grinding and milling with a wide array of crushers and mills. The crusher model is also supported in the batch environment in Aspen Plus.
- **Classifiers, Screens:** Adjust particle size distribution and identify with a range of classifiers and screens. The classifier model is also supported in the batch environment in Aspen Plus.
- **Separation:** Lower emissions of fine particles and reduce recycle streams using detailed solid-gas, solid-liquid and solids classification models.
- **Pneumatic Conveying:** Transport particles suspended in gas through a pipeline in either dense or dilute phase. Simulate a wide range of industrial applications.



## New Workflows

### One Flowsheet for Fluids and Solids

Aspen Plus is a simulation environment that unifies the modeling of solids and fluid processes. Aspen Plus includes an extensive model library for solids unit operations including drying, crystallization, granulation and agglomeration, crushing and grinding, classification, gas/solids and solid/liquid separation. In addition, an easy-to-use workflow for the definition of particle size distributions was introduced with an results representation that allows visualizing particle size distributions (e.g., cumulative, density or RRSB) and apparatus-specific results (e.g., separation efficiency curve of a screen or a gas cyclone) with the click of a button. Also, characteristic diameters such as  $d_{25}$ ,  $d_{50}$  or the Sauter Mean Diameter (SMD) are now shown in Aspen Plus in the stream results.

This enables the user of Aspen Plus, without any additional software use costs, to model processes that contain both fluids and solids in one simulation environment using consistent physical properties and avoid errors and inefficiencies that may result from the transfer of data from one simulation system to the other. Considering the entire process, rather than only smaller subsections, allows the user to avoid sub-optimal design due to localized optimization.

The need for combined fluid and solid process modeling is common for polymer processes. In Aspen Plus, there is an option to treat polymers and oligomers as solids under their melting points. Aspen Polymers, available in Aspen Plus, is the modeling technology for accurate and reliable optimization of polymerization processes. With this option, the polymer modeling capability is expanded to include purification, drying, and conveying, enabling more complete evaluations of both operational and process improvements. Figure 5 shows an example of this type of process.

### One Equipment Model from Conceptual to Rigorous

A single-unit operation can represent many different types of equipment at various levels of fidelity, from conceptual to rigorous. For example, a decanter centrifuge can be described by use of a conceptual model. In this case the user defines the split of the solids and liquid and the separation sharpness (slope of the separation curve), as shown in Figure 6. The model will then calculate a separation curve based on the settling velocity of the particles and the user input, as shown in Figure 7.

This means that already with the conceptual model the governing classification characteristic (in the present case, the settling velocity of the particles) is considered. If the user decides he needs to describe the centrifuge in more detail he can switch to the rigorous decanter model without changing the structure of the flowsheet or reconnecting streams to the block.

In the rigorous model, the user can define the geometry of the centrifuge and select from different options to describe the classification and the deliquoring that take place in the centrifuge. The centrifuge model will then calculate the separation efficiency curve based on the more rigorous model, so at a higher level of fidelity.

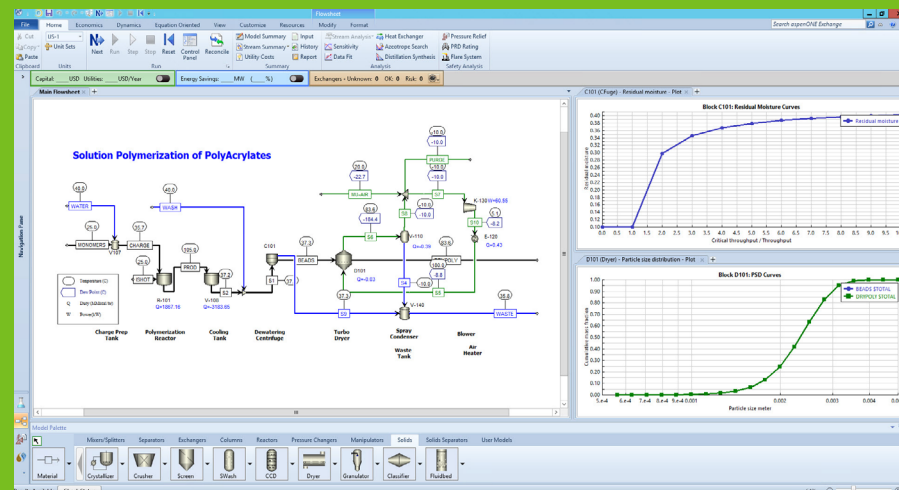


Figure 5: Polymerization and drying in one flowsheet, an example of a process with both a fluid and solid section

A comparison of the calculated separation efficiency curve using the conceptual and the rigorous model is shown on Figure 7. The plot shows that the conceptual model predicts the classification in the centrifuge with accuracy that already may be sufficient for different use cases, like for example a first feasibility study.

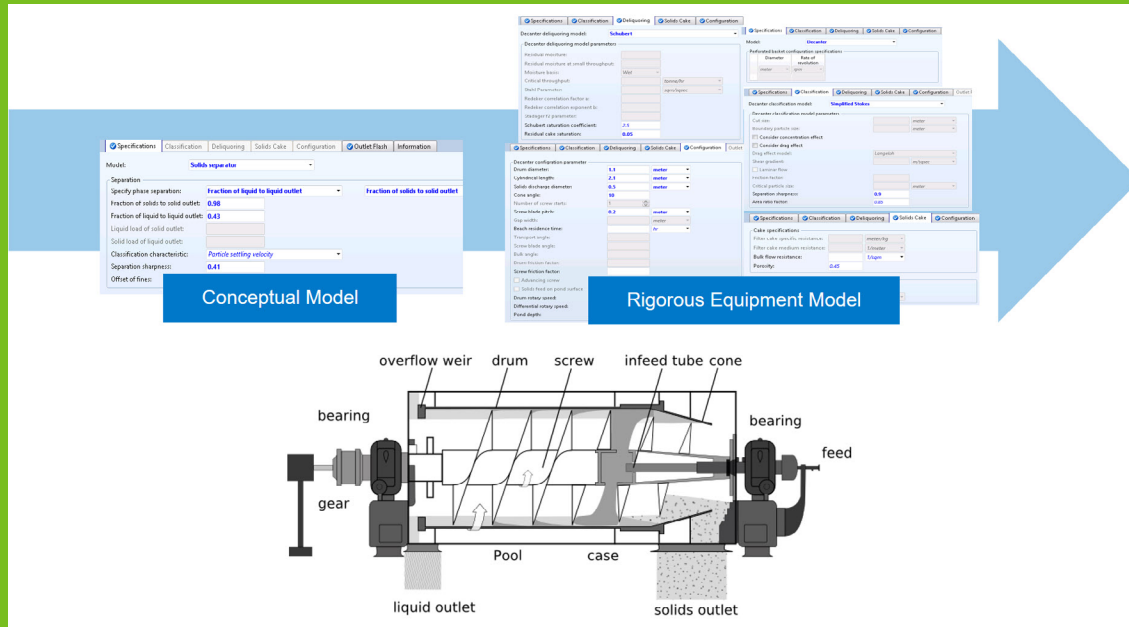
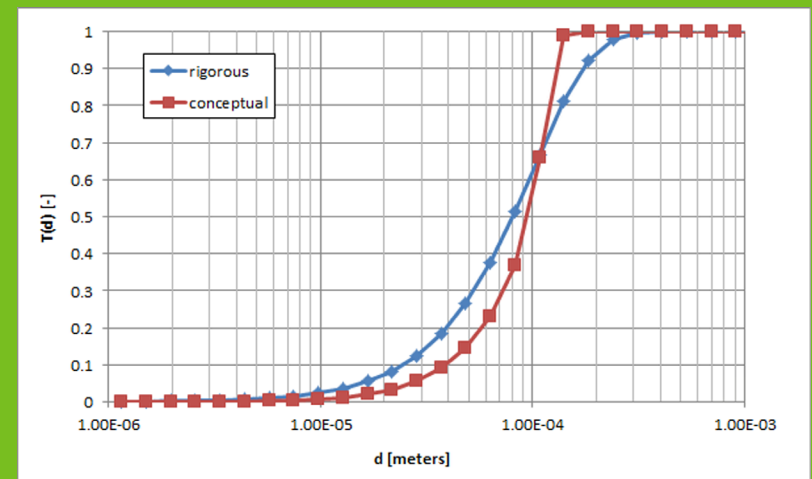


Figure 6: The screenshot on the left shows a decanter centrifuge described with a conceptual model, and the screenshots on the right shows the same decanter described with a rigorous equipment model.

Figure 7: Comparison of the calculated separation efficiency curve for the conceptual centrifuge model (red curve) and the rigorous decanter model (blue curve)





### **From Sequential to Simultaneous Conceptual Design**

Aspen Plus is surrounded by a suite of integrated products called aspenONE® Engineering. Aspen Plus supports integrated workflows such as activated Economic and Energy Analysis, as well as Exchanger Design and Rating (EDR). By modeling solids using Aspen Plus with aspenONE Engineering, users have access to these features and can optimize the energy demand of the entire process with activated energy. They can also access the effect on and troubleshoot capital and utility costs of solids modeling alternatives with activated economics. Using activated EDR, users can appropriately size heat exchangers required in the fluid part of the process.

Economics for solids allows users to consider the capital and utility costs for all solids processing blocks. The impact of design alternatives and their associated configurations and equipment specifications can be instantly seen.

### **Batch and Continuous**

Batch solids modeling operations are important for many industries. In Aspen Plus V10 and above, batch crystallization model is available in the BatchOp block. Additionally, the classifier and crusher blocks are supported in the batch environment in Aspen Plus.

With the crystallizer model, users can simulate continuous and batch crystallizers using a rate-limited nucleation/growth model based on super-saturation driving force. Users can also account for spontaneous nucleation, as well as growth from seed crystals, and consider concurrent reactions and crystallization. The flexible growth model allows for easy customization of rate expressions.



## Use in the Industry

Over 450 organizations have started using solids modeling in Aspen Plus, including the Dow Chemical Company. Dow engineers reported at AspenTech's OPTIMIZE® 2017 conference that they significantly improved their understanding of the solids behavior in a process involving solid reactants. They were also able to better understand the growth mechanism they were looking at and relate them with batch cycle time constants. This improved understanding helped them to optimize the entire process.

# Summary

Modeling solid processing steps using Aspen Plus V8 and above allows for improved workflow and collaboration between process engineers and particle scientists. Ignoring or poorly modeling the solids section of a process may lead to suboptimal designs and lost opportunities, such as reduced capital and operating costs and improved throughput and quality.

Modeling fluids and solids in one environment enables the optimization of the entire process at hand. Conceptual models further improve workflow for particle scientists and accessibility for process engineers that aren't savvy with solids process modeling — allowing users to create models of solids processing steps with only a few parameters.

The integrated workflow associated with using aspenONE Engineering stimulates better process designs and encourages more efficient collaboration. Processes that involve both batch and continuous process — including solids handling equipment — can be simulated in Aspen Plus.





AspenTech is a leading software supplier for optimizing asset performance. Our products thrive in complex, industrial environments where it is critical to optimize the asset design, operation and maintenance lifecycle. AspenTech uniquely combines decades of process modeling expertise with machine learning. Our purpose-built software platform automates knowledge work and builds sustainable competitive advantage by delivering high returns over the entire asset lifecycle. As a result, companies in capital-intensive industries can maximize uptime and push the limits of performance, running their assets faster, safer, longer and greener.

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