Frequently Asked Questions About Batch Modeling in Aspen Plus®

aspentech | FAQ

Batch Modeling in Aspen Plus enables quick and easy modeling of challenging batch processes, from development through product life cycle. By taking advantage of simulation, batch process industries can develop new processes faster, reduce experimental iterations during scale up and reduce batch cycle times.

This document answers some of the most frequently asked questions about this technology.

Q: What does Aspen Plus® offer for modeling batch distillation? What has changed from previous batch simulation solutions?

A: Batch Modeling in Aspen Plus offers quick and easy modeling of batch operations, including reactions, crystallization, drying, filtering and distillation—all from within Aspen Plus. From a single, integrated environment, users can:

- Simultaneously simulate batch, semi-batch and continuous processes
- Integrate batch models with custom and hybrid models
- Incorporate both solids and fluids
- Access the best-in-class physical property database

In addition to off-the-shelf models of common batch unit operations, users can insert a batch sub-flowsheet within a model that can solve dynamically. Sub-flowsheets define a sub-process that runs as a batch and can include both batch and peripheral equipment, such as condensers and decanters, which operate continuously. Finally, Batch Modeling in Aspen Plus provides informative, interactive graphics for batch distillation columns. From these graphics, users can view and edit rigorous geometry-based forms to define the column and dynamically plot changes in temperature, liquid levels and flow over time.

Previous versions of the aspenONE® Engineering suite provided batch simulation in both the standalone Aspen Batch Modeler and a batch reactor model (RBATCH) within Aspen Plus. Today all batch simulation capabilities have been fully integrated into Aspen Plus and are available as Batch Modeling in Aspen Plus. The integrated solution offers additional batch operations (e.g. crystallization), a batch sub-flowsheet, and enhanced graphics, while still supporting the previous RBATCH.

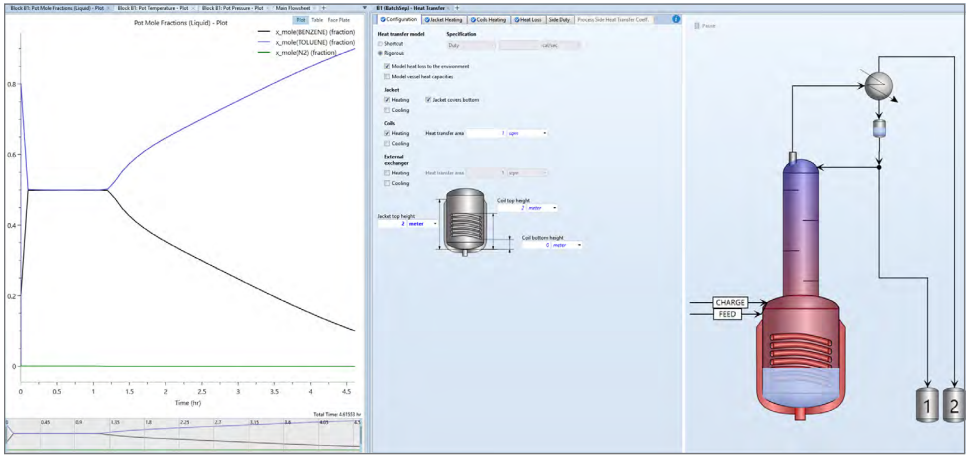


Figure 1. Dynamic plots capture time-lapse profiles or snapshots. Smart flowsheets animate during a run.

Q: Can I model batch reactors and reaction kinetics with Aspen Plus?

A: Yes. Aspen Plus V10 and above support batch operations, accessible as an off-the-shelf, configurable model. The batch operation model can be used standalone, in batch flowsheets and in batch sub-flowsheets. Batch sub-flowsheets are used to define a process within a larger process and can utilize both batch and continuous equipment within the larger process model.

The batch operation model can be configured for reactions, crystallization, drying and filtering. Moreover, one batch operation model can simulate more than one of these operations concurrently.

The batch operations model fully supports custom kinetics expressions (V12 and later) and fermentation kinetics (V14 and later). The legacy RBATCH unit operation is still available, for customers converting from an earlier Aspen Plus version or Aspen Batch Modeler.

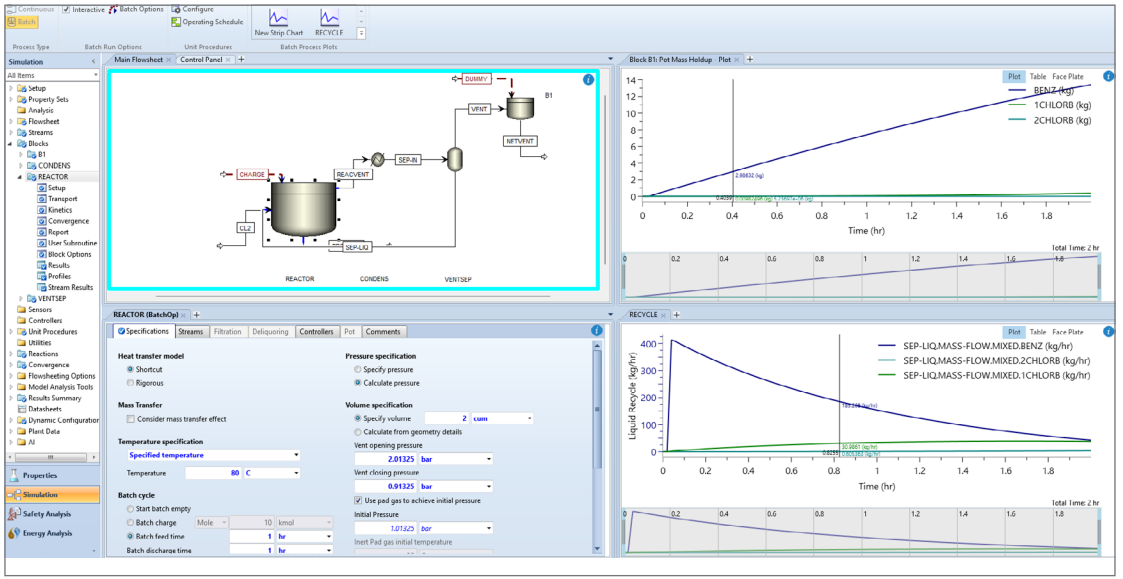
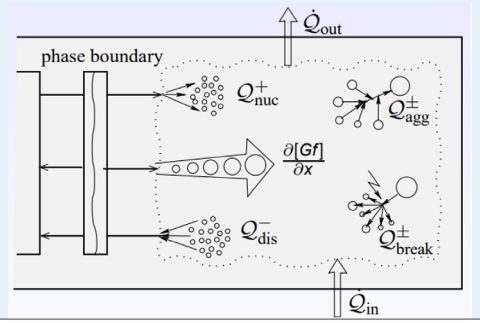


Figure 2. Users can easily flip between plot and table views of simulation results when using the batch operation model within Aspen Plus.

Q: Can I model batch crystallizers?

A: The batch operation, available in Aspen Plus V10 and later, supports continuous and batch crystallizers, with a rate-limited nucleation/agglomeration/growth model based on supersaturation as a driving force. Tailor the crystallizer model to your needs with a flexible growth model that allows for easy customization of rate expressions.

- Crystallization kinetics model using the "Reactions" feature in Aspen Plus
- Simulate continuous and batch crystallizers
- Rate-limited nucleation and growth model based on supersaturation driving force
- Option to account for **agglomeration**
- Account for spontaneous nucleation, as well as growth from seed crystals
- Flexible growth model that allows for easy customization of rate expressions
- Allow concurrent reactions and crystallization
- Track particle size distribution
- Simulate all modes of crystallization (evaporative, cooling, anti-solvent, etc.)



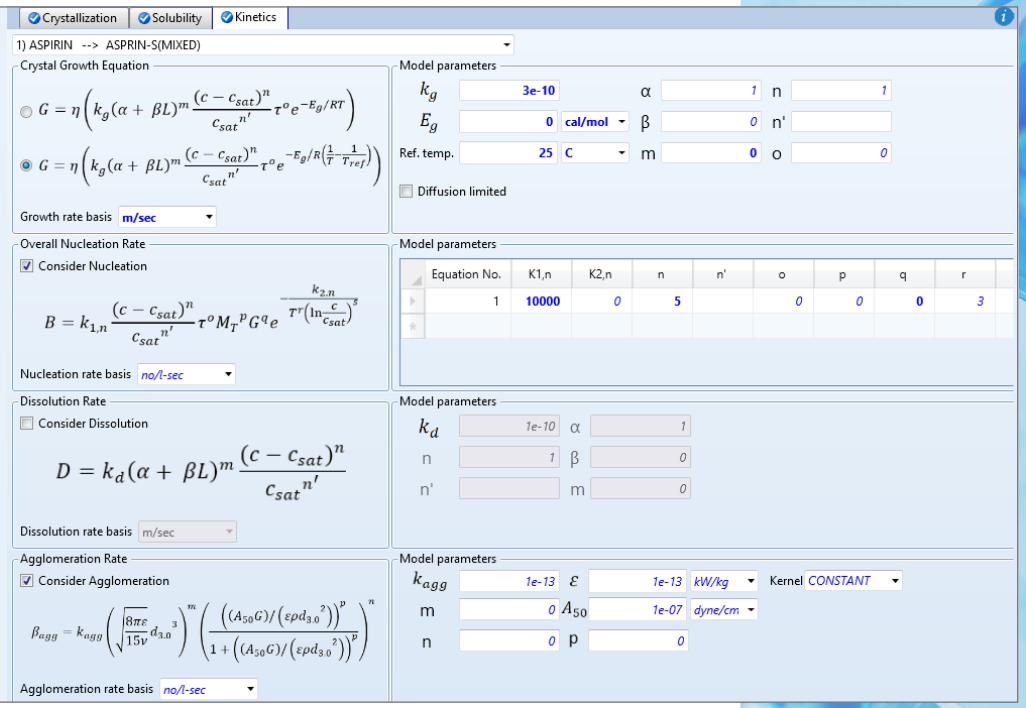


Figure 3. The crystallization model considers nucleation, growth, agglomeration and dissolution.

To learn more about Batch Crystallization in Aspen Plus, view this on-demand webinar:

Deliver Consistent Quality of Solids Using Crystallization Modeling

Q: Can I model a full batch process with multiple batch unit operations?

A: You bet! Aspen Plus V10 and higher allows users to configure batch sub-flowsheets. These sub-flowsheets can include multiple unit operations and can be integrated into a larger batch or continuous process. This can also be done with a batch distillation sub-flowsheet.

Many pre-defined equipment models are supported in these batch environments, including mixers and splitters, basic separation models, heater and heat exchangers, Stoichiometric and Gibbs reactor models, distillation columns, pumps, compressors, valves, dryers, solid operations, controllers, calculator and transfer operations, and hierarchy unit operations (to organize complex models), in addition to general batch operations.

Q: Can I model batch processes with continuous processes?

A: Many specialty, fine and life science processes involve both continuous and batch process sections. Ensuring maximum yield, minimizing operating costs or optimizing the product quality can be achieved with models that capture the entire process as opposed to single sections or units. Inside Aspen Plus V10 and above, you can simulate batch, semi-batch and continuous processes in the same model.

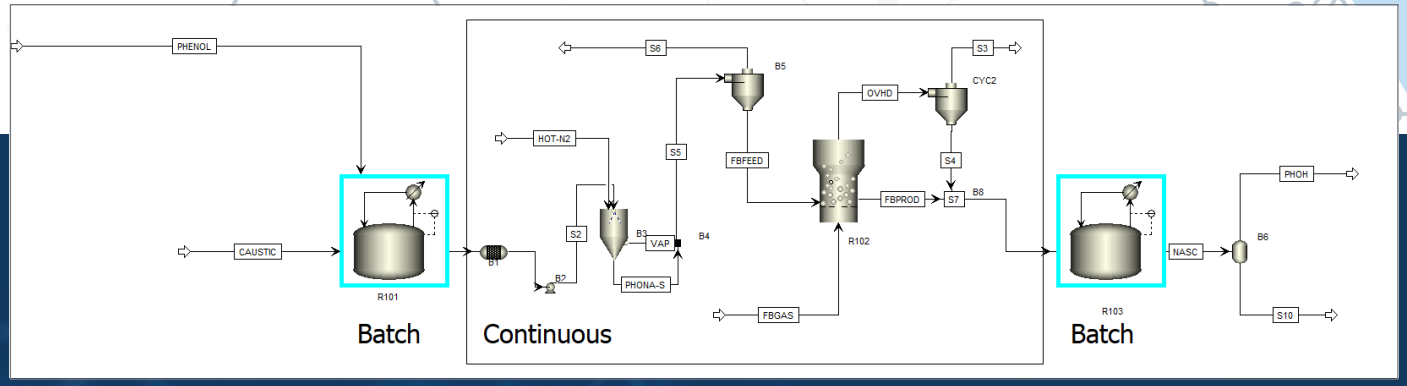


Figure 4. An example of an integrated batch/steady-state process. The main flowsheet is steady-state. Batch process sub-flowsheets (in blue borders) are solved dynamically by integration.

Q: Are there built-in physical properties? Can I estimate properties? Can I complete solubility analysis and solvent selection?

A: **Aspen Properties®**

From Aspen Plus, you can access Aspen Properties, the largest database of physical property data available. Complementing AspenTech's databases with the capabilities of NIST-TDE, Aspen Plus gives you access to data for 45,000 components, 127 property packages and over 5 million data points and interaction parameters. Employ state-of-the-art activity coefficient and equations of state models.

Estimating Capabilities, Customizable

Property databases can be customized and made private for intellectual property protection. Properties for unknown components can be estimated starting from a drawing of the molecular structure, and by using Aspen Plus property estimation capabilities. Experimental data can then be used for data regression.

Solubility Analysis Tool and Solubility Modeler

In addition to a powerful range of analysis tools (pure components or mixture properties), starting with V10, Aspen Plus includes a new Solubility Analysis tool for predicting solubility of components in solvent mixtures over a range of state conditions.

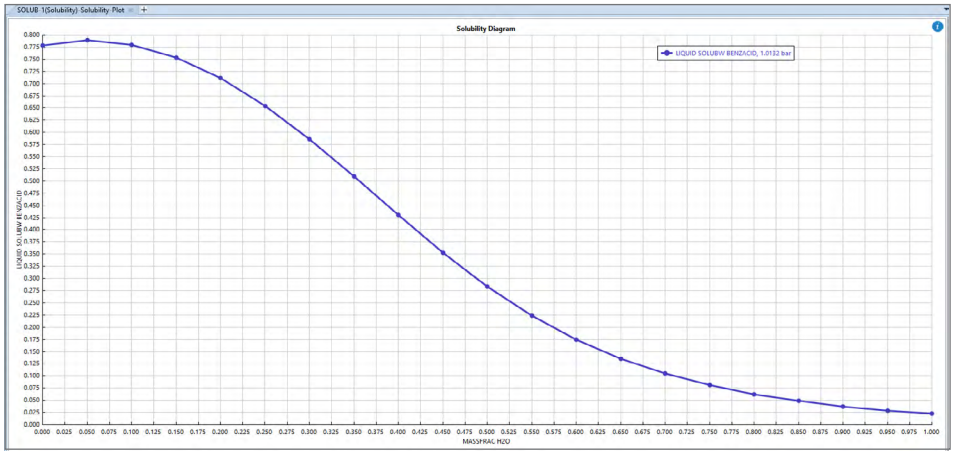


Figure 5. The new Solubility Analysis tool, available starting in V10 of Aspen Plus and Aspen Properties.

Q: I am new to modeling batch units and batch processes. What has AspenTech done to make this technology easier for me to use?

A: Integrating batch processes in Aspen Plus, a leading process simulation tool, eliminates the need to learn additional tools or integrate across multiple software environments. Moreover, Batch Modeling in Aspen Plus has an updated, modern user experience including:

- **Custom kinetics**. You can write algebraic expressions to define reaction kinetics. No need for FORTRAN or coding.
- **Definition of recipes.** Recipes can be defined through unit procedures, in a flexible approach that allows for a combination of parallel and series operations and use of multiple criteria to define every operation duration.
- **Visualization.** User can see a live update on block diagram, with temperature change and level fill in the tanks and visual geometry of the unit.
- **Operating Schedule.** Use Gannt-type diagrams to review the batch stages sequence and products results.

Aspen Plus also offers example models for a variety of use cases to help new users get started. These examples are available directly from Aspen Plus, under the Resources tab. From the Resources tab, users can also access Aspen Knowledge and the Support Center to find additional training resources.

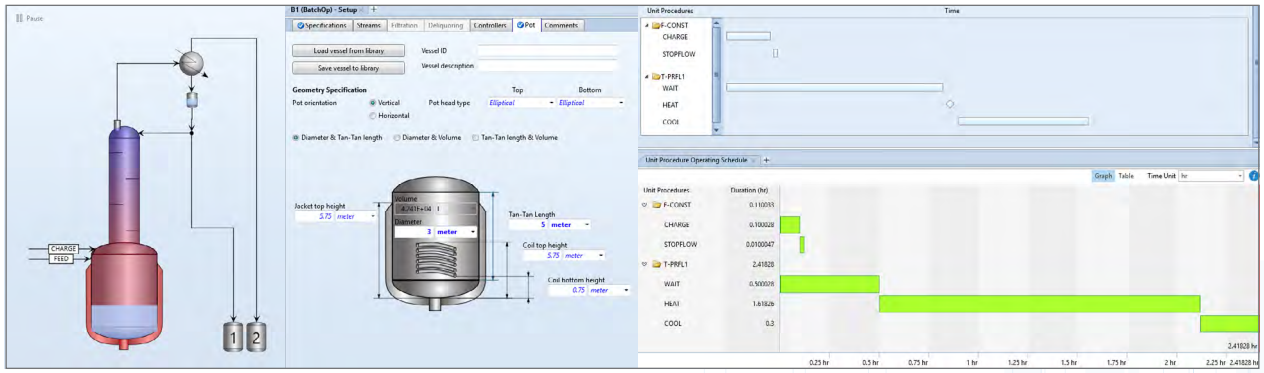


Figure 6. Batch distillation and operation visual geometry, Operating Schedule view.

User can visit:

- **AspenTech University** to learn more about training options and to search our knowledge base for published best practices, videos and more.
- **Aspen Plus Sustainability Applications** to view example models for sustainability applications.
- **AspenTech Support** for additional resources.

Q: Does Aspen Plus have sustainability or biobased component examples for batch modeling?

A: Yes. Aspen Plus provides many example models to be used as a starting point for modeling different processes. One example, a batch fermentation process to produce 1,4-butanediol (BDO) from glucose (or other renewable plant-based sugar feedstock), uses a batch reactor unit to model a fermentation reaction. Fermentation capability is available in Aspen Plus V14 and higher.

Another example uses AspenTech's batch reactor and fermentation kinetic models to develop a rigorous simulation of an anaerobic digestion process of biological waste to methane biogas. Multiple fermentation kinetic models are combined into a single reactor model to represent a wastewater treatment process involving mixed cultures of micro-organisms. The fermentation model provides sufficient flexibility to closely model real-world phenomenon. The models are capable of accurately predicting gas yield and gas production rates. This example can be used as a starting point for rigorous design and optimization of a wastewater treatment process.

Visit the **Aspen Plus Sustainability Applications website** to learn more about these and other sustainability examples.

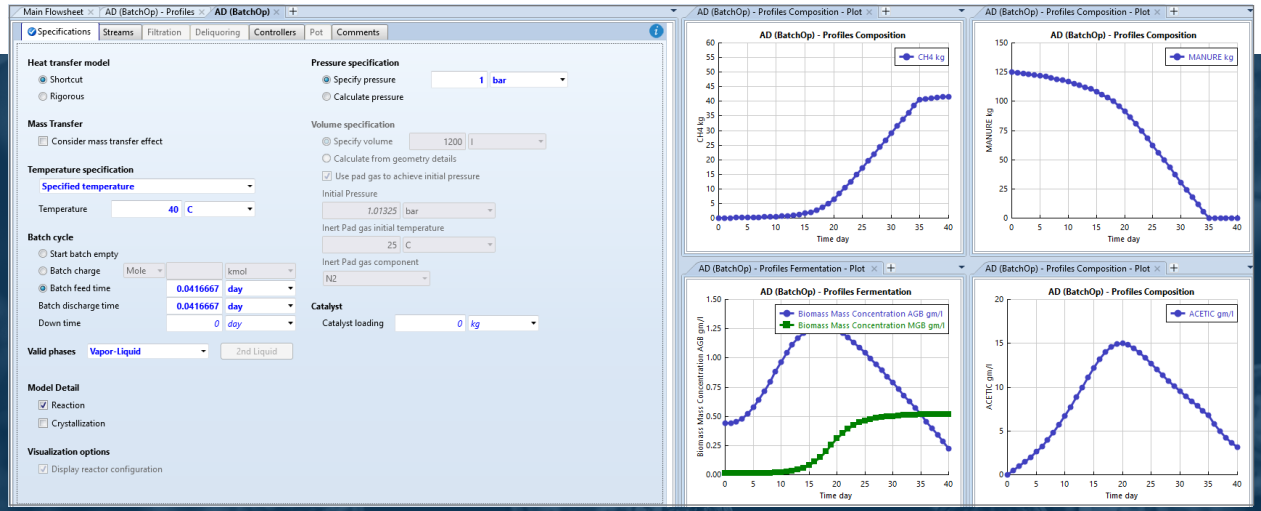


Figure 7. Example of a bioprocess in batch environment.

Q: Who is using this technology?

A: Dozens of organizations are using Batch Modeling in Aspen Plus. Here are a few examples of how organizations benefit from these capabilities.

Japanese Pharmaceutical Company Reduced Crystallization Time 96% and Decreased Impurities, While Investing Less Time in Process Design

Lubrizol Realized 10% Increase in Batch Capacity Without Needing Additional Capital Expenditure

Q: How do I get started using this technology?

A: **Webinars**

AspenTech regularly holds live one-hour webinars on various topics, and they are available on aspentech.com after the event.

Here is a list of relevant Aspen Plus webinars:

- **Webinar with Chemical Engineering: Accelerate Process and Product Development with Advanced Simulation**
- **Pfizer Accelerates Process Design and Scale-Up Using aspenONE Engineering**
- **Quick and Easy Batch Modeling Within Aspen Plus**
- **Maximize Batch Distillation Performance Using Aspen Plus**
- **Simplify Batch Process Improvement Using Aspen Plus**
- **Deliver Consistent Quality of Solids Using Crystallization Modeling**

Q: How-to Videos

- Several how-to videos are available on the **AspenTech Support Site.**

Didn't see your question here? **Contact Us** to talk directly to an AspenTech representative.

About Aspen Technology

Aspen Technology, now part of Emerson, is a global software leader helping industries at the forefront of the world's dual challenge meet the increasing demand for resources from a rapidly growing population in a profitable and sustainable manner. AspenTech solutions address complex environments where it is critical to optimize the asset design, operation and maintenance lifecycle. Through our unique combination of deep domain expertise and innovation, customers in asset-intensive industries can run their assets safer, greener, longer and faster to improve their operational excellence.

www.aspentech.com