

Many new improvements have been made to Batch Modeling technology in Aspen Plus, including the integration of the technology previously available with Aspen Batch Modeler and the introduction of new unit operations, including batch crystallization. This document covers our answers to some of the most commonly asked questions about this technology.

# 1. What does Aspen Plus offer for modeling batch distillation? BatchSep for Modeling Batch Distillation

In Aspen Plus, all batch distillation modeling technologies have been fully integrated and enhanced starting with V10. In previous versions of the aspenONE® Engineering suite, the technology was available in the standalone Aspen Batch Modeler, as well as with the BatchSep block within Aspen Plus. The forms in BatchSep have been optimized from a user experience standpoint and include interactive informative graphics, such as unit configuration, liquid levels, temperatures and flows. Reactions and multiple stop criteria are fully supported.

Aspen Plus users can click on the graphic to view and edit the rigorous geometry-based input forms. These interactive graphics are dynamic, showing temperature and levels over time.

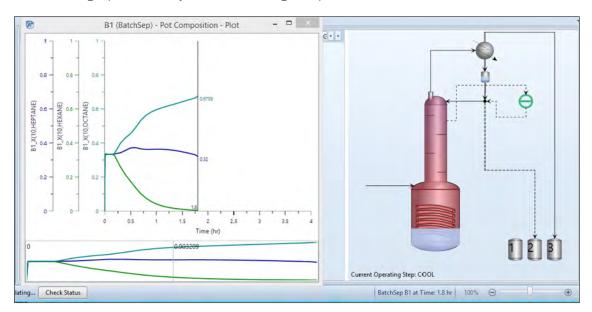


Figure 1: New dynamic plots capture time-lapse profiles or snapshots.
Smart flowsheets animate during a run.

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

### **Maximize Batch Distillation Performance Using Aspen Plus**

#### 2. Can I model batch reactors and reaction kinetics with Aspen Plus?

The new BatchOp unit operation available in Aspen Plus V10 and above can be used for modeling both reactors and crystallizers. BatchOp can be used inside batch flowsheets including the BATCHPROCESS container.

#### BatchOp for Modeling Reactors

In Aspen Plus, we recommend the BatchOp unit operation for modeling batch reactors as standalone unit operations or as part of an entire batch process; the legacy RBatch unit operation from previous versions of Aspen Plus is still available. Use BatchOp to model batch reactions and crystallization — also concurrently. Take advantage of the reaction models and physical properties database in Aspen Plus to scale up your process. BatchOp fully supports custom kinetics expressions (NEW in V10).

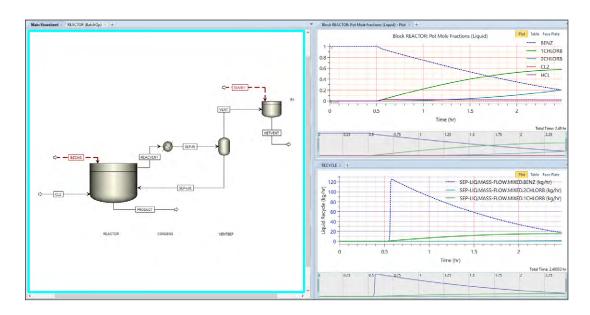


Figure 2: New plotting capabilities were added with the new BatchOp unit operations, including the ability to flip between plot and table views of results.



### 3. Can I model batch crystallizers?

### BatchOp for Modeling Batch Crystallizers

Starting with V10 of Aspen Plus, you can simulate continuous and batch crystallizers with a rate-limited nucleation/growth model based on supersaturation as a driving force. Batch crystallizers can be simulated in BatchOp. Account for spontaneous nucleation as well as growth from seed crystals and allow concurrent reactions and crystallization. Tailor the crystallizer model to your needs with a flexible growth model that allows for easy customization of rate expressions.

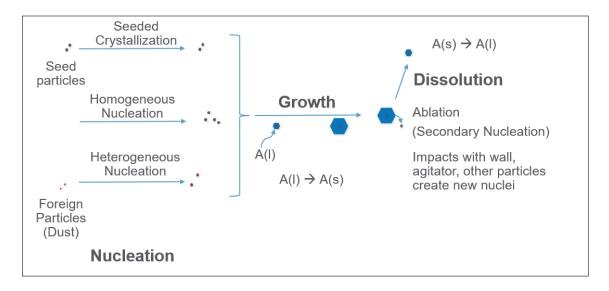


Figure 3:
The crystallization model considers nucleation, growth and dissolution.

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

**Deliver Consistent Quality of Solids Using Crystallization Modeling** 

#### 4. Can I model a full batch process with multiple batch unit operations?

You bet! Starting in V10, Aspen Plus includes a new block called BATCHPROCESS, a configurable sub-flowsheet that can include multiple unit operations and that can be used in the context of an integrated batch/continuous process. BatchSep, a batch distillation sub-flowsheet, was also improved in V10.

Many blocks are supported in these batch environments, including mixers & splitters, basic separation models, heater & heat exchanger, RStoic and RGibbs reactor models, pumps, compressors, valves, solid operations, BatchOp (general purpose batch operation), controllers, calculator & transfer blocks and hierarchy blocks (to organize complex models).

To learn more about Aspen Plus for batch modeling, view these webinars:

**Quick and Easy Batch Modeling within Aspen Plus Simplify Batch Process Improvement Using Aspen Plus** 

### 5. Can I model batch processes with continuous processes?

Many specialty, fine and life science processes involve both continuous and batch process sections. Ensuring maximum yield of the most valuable product, 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.

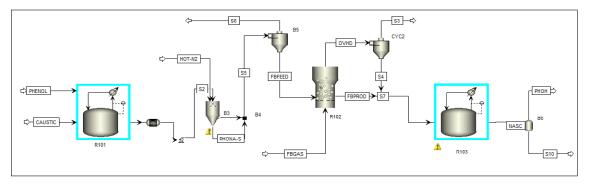


Figure 4: An example of an integrated batch/steady-state process. The main flowsheet is steady-state. Batch process sub-flowsheets (in aqua-blue borders) are solved dynamically by integration.

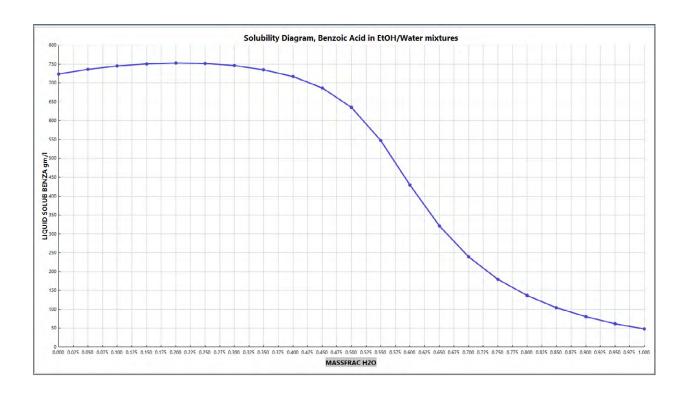


Figure 5: The new Solubility Analysis tool available starting in V10 of Aspen Plus

# 6. Are there built-in physical properties? Can I estimate properties? Can I complete solubility analysis and solvent selection? Aspen Properties

With Aspen Plus, you have access to 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 37,000 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.

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

Batch process improvement technology has an updated, modern user experience with its integration into Aspen Plus. Here are a few improvements that we think you will enjoy if you are a new user (or an existing one):

- 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 forms, in a flexible approach that allows for a combination of parallel and series operations and use of multiple criteria to define every operation duration.

# 8. As part of my process development efforts, I want to evaluate the implications of scaling up my recipe. Does AspenTech have a tool for this?

Yes, Aspen Batch Process Developer™ is a recipe-based modeling technology for batch process scale-up, and is used for developing batch process models from early route selection to full-scale manufacturing.

To learn more about **recipe-based process scale-up**, visit AspenTech.com.

### 9. Who is using this technology?

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

**Qenos:** Engineers at Qenos realized savings of \$135,000 USD per year and completed plant trials for a new product grade six months ahead of schedule.

The Dow Chemical Company: Dow achieved a 25 percent reduction in batch cycle time.



### 10. How do I get started using this technology?

#### Webinars

AspenTech regularly holds live one-hour webinars on various topics, and they are available on our site after the event. Here is a list of relevant Aspen Plus webinars:

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** 

#### How-to Videos

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

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

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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