

Aspen Hybrid Models™ V12

November 2020

Technology Overview

What are Aspen Hybrid Models?

Hybrid models combine AI and first principles to deliver a comprehensive, accurate model more quickly without requiring significant expertise. Machine learning is used to create the model leveraging simulation or plant data, while using domain knowledge including first principles and engineering constraints to build an enriched model without requiring the user to have modeling expertise or become an AI expert.

Aspen Tech is uniquely positioned to leverage over 40 years' domain expertise to make AI applicable to process industries. This next generation of solutions will democratize the application of AI with Aspen Hybrid Models to optimally design, operate and maintain assets—online and at the edge.

What is the advantage of Aspen Hybrid Models over traditional AI?

We are focusing on managing constraints: we apply domain knowledge to ensure models are giving reasonable closure for mass, energy and atom balances. This allows the models to be used in the context of Aspen Plus®, Aspen HYSYS® and Aspen PIMS-AO™ without loss of information. This is a big advantage over generic AI modeling tools which will allow infeasible solutions.

What are the benefits of Aspen Hybrid Models?

With Aspen Hybrid Models, companies can model processes and assets that cannot easily be modeled with first principles alone. You get the accuracy of empirical models and the strength of first principles models, leveraging the power of AI, along with 40 years of domain expertise, to create a more predictive model.

With Aspen Hybrid Models, organizations can create better performing models that will allow them to do more frequent analysis and obtain greater benefits continuously. Aspen Hybrid Models help companies to create and sustain better models, faster. They provide a better representation of the plant, which keeps the model more relevant over a longer period of time.



Use Cases and Application of Aspen Hybrid Models

What are the main applications for Aspen Hybrid Models?

Aspen Hybrid Models have many applications across all verticals. In summary, use cases can be grouped in the following categories:

- Operations Optimization
 - Fast offline and online models
 - Rapid planning update
 - Nonlinear planning models
- Soft sensors for product and operations KPIs
 - New properties such as color and polymer melt index
 - Better oil and gas properties
- New equipment models
 - Complex reactor models
 - New types of columns
 - Other existing equipment
- Fast asset-wide models
 - Integrated upstream and midstream facilities
 - Integrated oil to chemicals
 - Site-wide optimization
 - Site-wide models for emission monitoring



What are some of the applications of Aspen Hybrid Models in upstream and midstream?

Some use cases include:

- Oil & gas separation
- Hydrate formation and inhibition
- Property sensors (pH, Reynolds)
- LNG plant
- Natural gas dehydration
- Sales gas dew point
- Compressor trains
- CO₂ freeze temperature

What are some of the applications of Aspen Hybrid Models in refining?

Some use cases include:

- Crude distillation unit
- Hydrocarbon dew point
- BTX separation
- Sour water stripper
- Fluidized bed reactor
- Reformer reactor
- Hydrogenator
- Reactor relief pressure
- Coke calcination
- Assay property sensor
- Reactor models for engineering and planning

What are some of the applications of Aspen Hybrid Models in bulk chemicals?

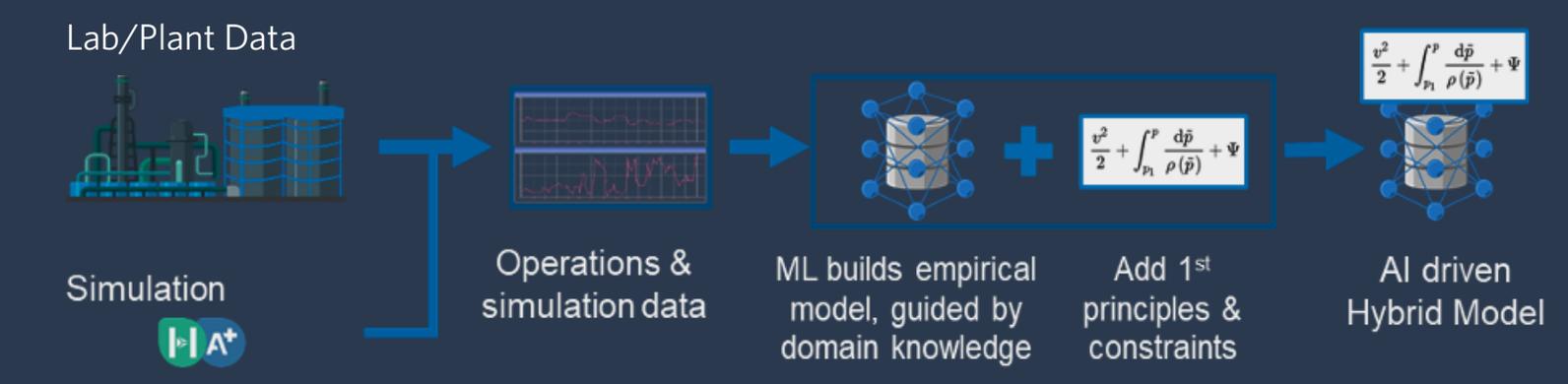
Some use cases include:

- Methanol synthesis
- Propane dehydrogenation
- Propylene glycol
- Cumene
- Methylcyclohexane
- Terephthalic acid
- Distillation
- Fluidized bed
- Convective heat transfer
- Ammonia synthesis
- Reactor models
- Cracked-gas compression

What are some of the applications of Aspen Hybrid Models specialty chemicals and polymers?

Some use cases include:

- Crystallization & drying
- Membrane
- HDPE polymerization
- Centrifuge
- Crusher
- LDPE polymerization
- Polyolefin purge
- Polymer attributes
- Polymer hardness
- Drum filter
- Polymer melt index



Types of Aspen Hybrid Models

What are the different types of Aspen Hybrid Models available in V12?

There are two different types of Aspen Hybrid Models:

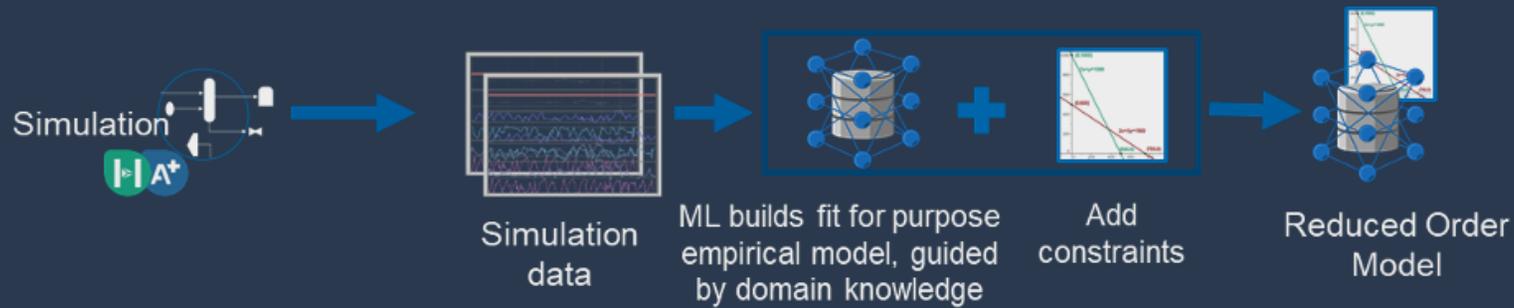
- AI-Driven Hybrid Models
- Reduced Order Hybrid Model

What is an AI-Driven Hybrid Model?

In this approach, machine learning is used to create an empirical model based on plant or experimental data, augmented with first principles (e.g. Reynolds number etc.), constraints (e.g. mass balance) and domain knowledge to create the resulting hybrid model. This approach allows a less experienced user to rapidly generate a completely new predictive, more accurate model, fully democratizing AI's application. Users can now model processes and assets that cannot easily be modeled with first principles alone.

Some examples include:

- Complex process units and processes
- Inferential sensors
- Equipment unit models online



What is a Reduced Order Hybrid Model?

In this approach, machine learning is used to create an empirical model based on data from numerous simulation runs, augmented with constraints (e.g. mass balance) and domain expertise, to build a fit for purpose, high fidelity, performant model that is accurate within the range for which it has been trained, fully democratizing the application of AI. With reduced order models the user can easily extend the scale of modeling from units to the entire site and can synchronize the model across design, operations and maintenance.

Some examples include:

- Refinery-wide or chemical plant-wide models
- Planning model updating
- Fast-solving online models to predict best/worst-case schedules for cleaning
- Process train models online

Can the different types of Aspen Hybrid Models work together?

Yes. The different models are not mutually exclusive. For example, a user can have a site-wide reduced order model, with AI driven sensors to account for key properties, such as emissions. Or users can have AI-driven equipment models in a simulation, and then create a reduced order model that can be deployed in planning or for online applications.



What are the components necessary to use Aspen Hybrid Models?

The two main components of Aspen Hybrid Models involve the workflows to create and deploy the model. First, the model is created using Aspen AI Model Builder™, a SaaS application running in the Aspen cloud. After the model is created, it can be deployed to applications such as online digital twins, Aspen HYSYS and Aspen Plus for engineering and debottlenecking, and Aspen PIMS-AO for planning.

Which products and versions support Aspen Hybrid Models?

Aspen Hybrid Models can be deployed directly in both Aspen HYSYS and Aspen Plus V12. It is also possible to deploy in Aspen HYSYS and Aspen Plus V10 and V11 with some additional steps. Models can also be used in conjunction with Aspen OnLine™ for Digital Twin applications or deployed in Aspen PIMS-AO for updating non-linear planning models.

What are the different steps to create a hybrid model?

Aspen Hybrid Models are created using Aspen AI Model Builder. This application enables users to define and collect data from different sources (plant data, simulation data, Aspen Multi-Case™, etc.), aggregate data, model data, apply insights and create the model to be deployed to the different products: Aspen HYSYS, Aspen Plus or Aspen PIMS-AO.

Creating Aspen Hybrid Models in Aspen AI Model Builder

Do I need Aspen Multi-Case to create a model in AI Model Builder?

Aspen Multi-Case uses parallel computing to run hundreds of simulation cases concurrently. It is not required but it will significantly speed data generation for building Reduced Order Hybrid Models.

Are there features that help provide confidence in the model's accuracy?

We are looking at ways to improve the interpretability of the model without exposing our hybrid modelling intellectual property. After models are created, AI Model Builder shows parity plots that display accuracy and predictability of the model based on test and train data. In the AI-driven workflow, we display a coefficient plot, which includes the terms in the equation and the relative value of the coefficients. The user can review information on the coefficient plot to better understand what values have an impact on the dependent variables and then build confidence in the results. While the underlying algorithms are not displayed, Aspen AI Model Builder includes data cleaning methods to improve the quality of data used to create the model, ensuring a highly predictive model that users can trust.

How do Hybrid Models and Aspen Multi-Case handle convergence issues?

If the model is well structured, there should not be any trouble to run multiple cases to generate the data to create the model. When the data is exported from Aspen Multi-Case, any cases that did not converge will be eliminated from the data set.

When you deploy into Aspen Plus or Aspen HYSYS, the model uses the same conversion strategy already built in the simulator. If the model has recycle loops and they are created within the Reduced Order Model, this will not present a convergence issue.

What is an advantage of not displaying the data used to create an Aspen Hybrid Model?

Technology suppliers and licensors can create Aspen Hybrid Models out of their proprietary technology and share these models to customers and end users without exposing proprietary information. As data is used to create the model, Aspen AI Model Builder helps to build confidence in the results. During deployment, this data is protected when the model is created and used.

When AspenTech updates the SaaS product, will previously-created models work the same?

In Aspen AI Model Builder, the algorithm displays a version, so with any change, the user can evaluate the performance of an existing project with the different versions of the algorithm and decide which one to choose. This is designed to let users quickly compare the results without having to go through the complete design of experiments.



How is the security addressed when updating data to the cloud?

All users have a unique login, where nothing can be shared between different users. For login, we use two-factor authentication to improve security. Aspen AI Model Builder also uses https. And all data is stored in a third-party object storage service that uses the latest security protocols.

Are services required to create and implement Aspen Hybrid Models?

Aspen AI Model Builder was designed so users can build the models by themselves. Data science expertise is not required to apply AI in the process industry and obtain the most value from the technology. For more complex scenarios and higher sophistication, AspenTech

services and ISPs are fully trained to provide the help needed to create and deploy the models. When models are deployed, they can be used by any of our typical users: a process engineer, planner, control engineer, etc.

As most data is generated in steady state, you may reproduce the normal operation but not the perturbances. How do you deal with this?

Our guidance is to build a model using a training dataset containing as much variance as possible. This dataset should ideally cover a wide range of different operating conditions, including steady state conditions and disturbances. It may also be possible in some applications to supplement these data with simulation data to cover regions where plant data is sparse.

Deploying Aspen Hybrid Models

What are the workflows available in V12 to deploy Aspen Hybrid Models?

The three workflows available are:

- Reduced Order Hybrid Models deployed to engineering
- AI-Driven Hybrid Models deployed to engineering
- Reduced Order Hybrid Models to planning





A Reduced Order Hybrid Model can be deployed to Aspen HYSYS and Aspen Plus as a sensor or as equipment, where equipment refers to either a single piece of equipment or an entire flowsheet. AI-Driven Hybrid Models can also be deployed to Aspen HYSYS and Aspen Plus as sensors or equipment. Reduced Order to planning will create a non-linear planning sub-model to be used in the Aspen PIMS-AO refinery model.

How can you deploy an Aspen Hybrid Model online?

Aspen Hybrid Models deployed to Aspen HYSYS and Aspen Plus can be used in steady state models as digital twin applications through Aspen OnLine and Aspen Plant Data.

Aspen OnLine can access the deployed Hybrid Model in Aspen HYSYS and Aspen Plus V10, V11 and V12. In Aspen HYSYS and Aspen Plus V12, users have a complete workflow to deploy online models using plant data, where through the same process modeling environment, they are able to create the process flowsheet, calibrate models with plant data and generate models for online deployment.

How do you test the accuracy of the results in areas where there is no plant data available?

Since the hybrid model is only trained and tested in areas where you have supplied data, we are unable to guarantee accuracy in regions with no plant data. The model will still solve but you will get a warning that the model has solved outside of the training bounds.

General Questions

Can I install these tools on a local machine or do they need to be on a server?

Aspen Multi-Case is a desktop tool, like the rest of the Engineering suite. You can run it locally on your own computer or it can run in a high-performance server shared by many people. Aspen AI Model Builder is a cloud-based product deployed in the Aspen Cloud, which means that does not need any local installation.



What is the difference between sensor and equipment models?

An inferential sensor, virtual sensor or just “sensor” is deployed in Aspen HYSYS or Aspen Plus to predict properties inside your design or your operations model. It can predict properties such as viscosity, color, porosity or permeability and is linked to streams or equipment in the simulation environment.

A sensor model can also be used to represent unit operations, and provides more simulation flexibility, especially in cases where not all variables such as temperature, pressure or composition are known.

A Hybrid Model equipment represents a piece of equipment such as a reactor or a membrane. It can also represent a section of a flowsheet

or a complete flowsheet that can be used for site-wide analysis or for applications such as modeling the integrated oil to chemicals process. Unlike sensor hybrid models, equipment hybrid models are deployed on the simulation environment and can be connected to material streams in the flowsheet environment.

What is the difference between Aspen Hybrid Models and custom models?

One of the goals of Aspen Hybrid Models is to democratize the use of machine learning technology to enable process engineers to use these powerful methods without being experts in data science. We also take advantage of our plant data infrastructure, enabling efficient data collection and cleaning.

Hybrid Models provide an alternative to first principle custom models by leveraging large amounts of data. There will still be a place for custom models as well. First principle custom models take advantage of our knowledge of science and engineering to develop predictive models even when very limited data is available.

Have more questions? [Contact support](#) or visit our [Aspen Hybrid Models web page](#)

About Aspen Technology

Aspen Technology (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 safer, greener, longer and faster. Visit [AspenTech.com](https://www.aspentech.com) to find out more.

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