

Aspen Hybrid Models™ V12.1  
May 2021

# Technology Overview

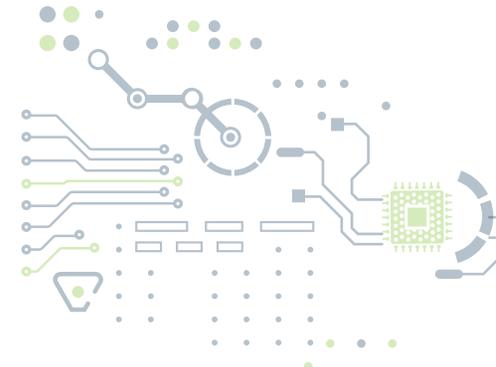
## What are Aspen Hybrid Models™?

Aspen 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 the need for modeling or AI expertise.

This next generation of solutions democratizes the application of AI with Aspen Hybrid Models to optimally design, operate and maintain assets—online and via edge—enabling you to model processes and assets which cannot easily be modeled with first principles alone.

Aspen Hybrid Models combines the accuracy of empirical model, the strength of first principles models, and the power of Industrial AI, leveraging our 40 years of industry and domain expertise to create a more predictive model.

This technology allows organizations to create a better performing model, perform more frequent analysis and continuously obtain greater results. Aspen Hybrid Models provides an end-to-end workflow to create and sustain more accurate, longer-term models.



### **What benefits could an engineering firm expect from Aspen Hybrid Models' adoption?**

Benefits of traditional online and offline modeling can be extended through hybrid modeling to cases where models are not available or easy to run today. This technology can help companies to accurately simulate equipment, processes and KPIs—defining and implementing strategies to increase yield (1-5%) and throughput (5-10%) or reduce energy demand (5-20%) in a range of assets from single units to large and integrated sites.

### **What might the expected benefit be from Aspen Hybrid Models' adoption in planning?**

Planning model accuracy can be increased by over 97 percent, helping helping organizations make better business decisions and increase refinery margins. With the end-to-end workflow combining engineering's rigorous reactor models and a planning submodel, updates can be performed in at least half the time.

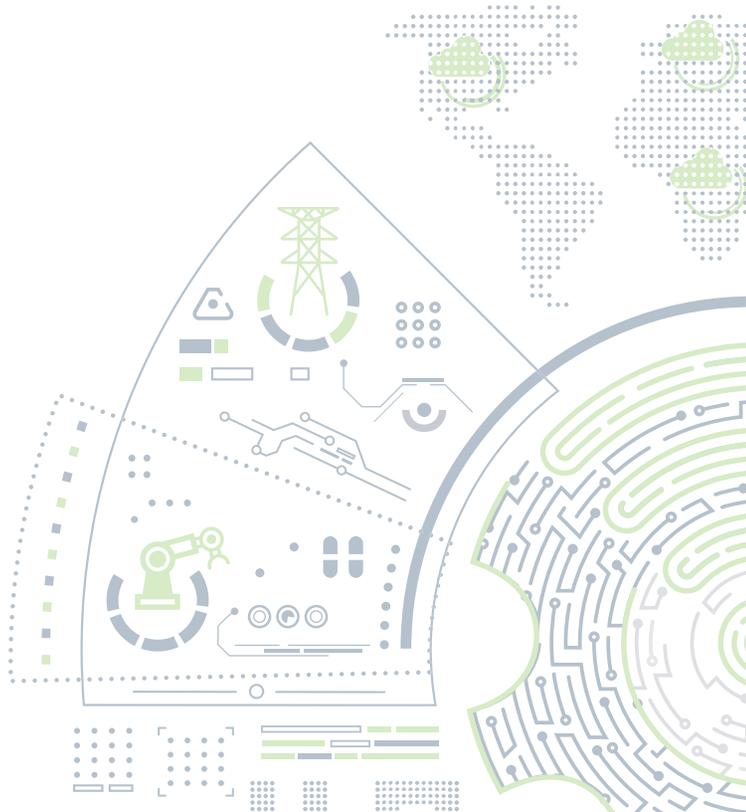
### **How do Aspen Hybrid Models assist control and optimization?**

High fidelity unit optimization models enable model alliance between process engineering, planning and process control.

Nonlinear optimization with these models increase accuracy of the optimization, leading to increased profits and reduced margin leakage.

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

With a focus on managing constraints, we leverage our domain knowledge to ensure our models are providing reasonable closure for mass, energy and atom balances. This allows the models to be used in the context of Aspen Plus®, Aspen HYSYS®, Aspen PIMS-AO™ and Aspen Unified™ without loss of information—a big advantage over generic AI modeling tools which enable infeasible solutions.



# Use Cases and Applications of Aspen Hybrid Models

## What are the main applications for Aspen Hybrid Models?

Aspen Hybrid Models have many applications across all verticals. Use cases can be grouped into the following categories:

### ■ Operations Optimization

- Fast offline and online models
- Rapid planning update
- Nonlinear planning models

### ■ Fast asset-wide models

- Integrated upstream and midstream facilities
- Integrated oil to chemicals
- Site-wide optimization
- Site-wide models for emission

### ■ 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

### ■ Model real equipment performance

- Column efficiencies
- Reaction rates
- Heat transfer coefficients
- Pipeline friction factors





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

- Oil and gas separation
- Hydrate formation and inhibition
- Property sensors (pH, Reynolds)
- LNG plant
- Natural gas dehydration
- Sales gas dew point
- Compressor trains
- CO<sub>2</sub> freeze temperature

### What are the primary applications of Aspen Hybrid Models in refining?

- 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

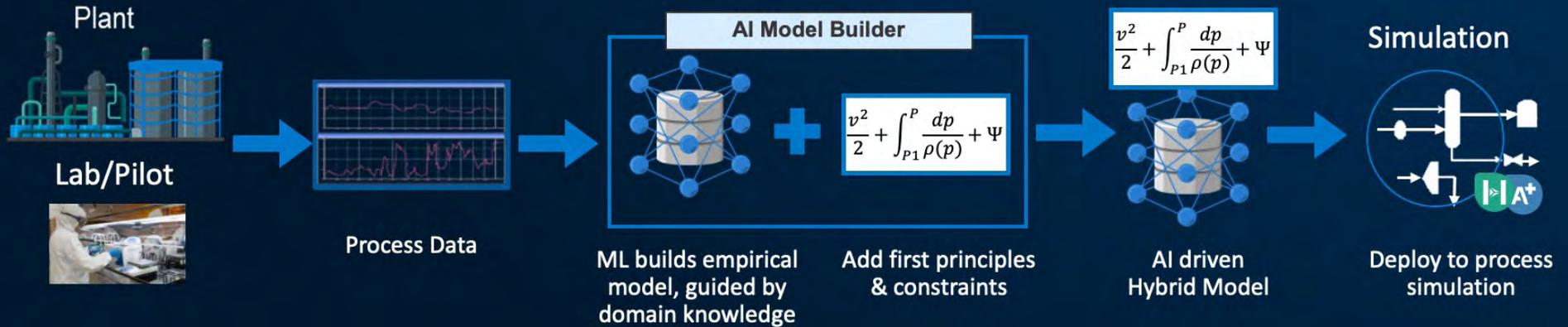
### What are the primary applications in bulk chemicals?

- 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 in specialty chemicals and polymers?

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

## AI-driven Hybrid Models



## Types of Aspen Hybrid Models

### What are the different types of Aspen Hybrid Models?

- AI-driven Hybrid Models
- Reduced Order Hybrid Model
- First Principles-driven Hybrid Models

### 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), constraints (e.g. mass balance) and domain knowledge to create the resulting hybrid model.

The AI-driven approach enables a less experienced user to rapidly generate a brand new predictive, more accurate model, fully democratizing AI's application. This means that processes and assets which cannot easily be modeled with first principles alone can now be modeled.

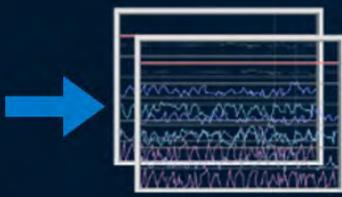
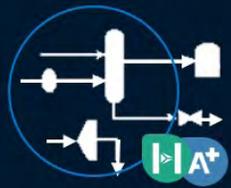
Some examples include:

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

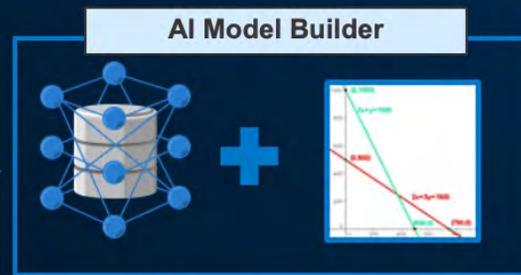


## Reduced Order Hybrid Models

### Simulation

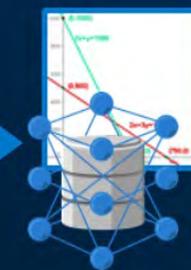


Simulation Data



ML builds fit –for-purpose, simple and more robust model

Add constraints



Reduced Order Hybrid Model



Deploy to multiple applications

### 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. Machine learning builds 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, you can easily extend the scale of modeling from units to the entire site and synchronize the model across design, operations and maintenance.

Some examples include:

- Refinery-wide or chemical plant-wide models
- Nonlinear planning model update with seamless end-to-end workflow
- Fast-solving online models to predict best/worst-case schedules for cleaning
- Process train models online
- Dynamic optimization of complex reactors

### What is a First Principles-driven Hybrid Model?

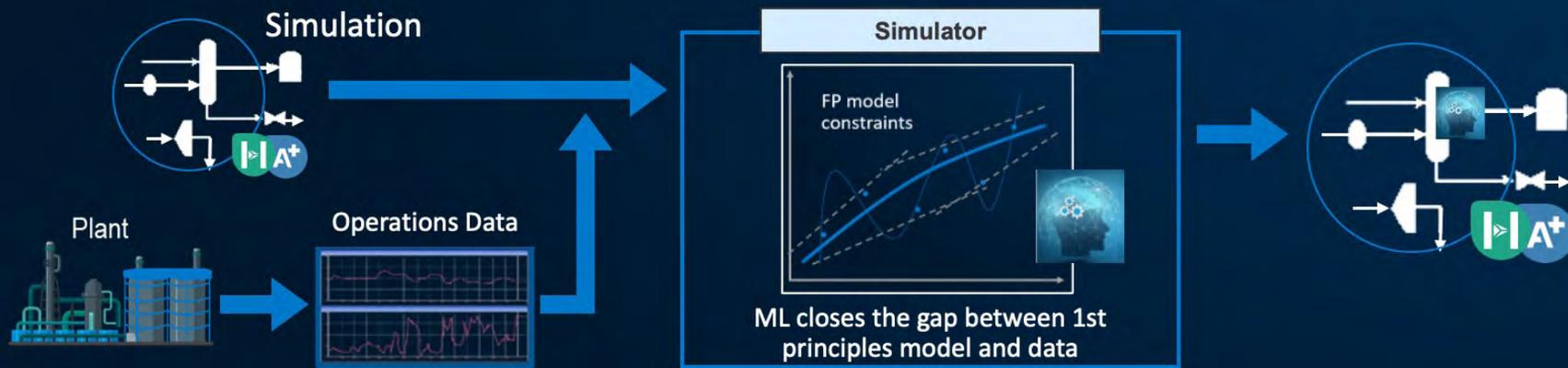
With the first principles-driven type of Aspen Hybrid Model, an existing first-principles model is enhanced using AI with data from operations to calculate unknown variables and relationships not captured by the original model (e.g., reaction rates). Machine learning is used to determine the unknown value and its relationships to continuously calibrate the model as conditions change. This approach is a natural extension to existing first principles models in many brownfield deployments globally; it is quick and easy to adopt and significantly increases model accuracy.

Some examples include:

- Column efficiencies
- Reaction rates
- Bioprocess reactors
- Modeling complex units



## First Principles-driven Hybrid Models



### Can the different types of Aspen Hybrid Models work together?

Yes. The different types of models are not mutually exclusive. For example, you can have a sitewide reduced order model with AI driven sensors to account for key properties, such as emissions. Or you can have AI-driven or First Principles-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 different steps to creating a hybrid model?

AI-driven and Reduced Order Hybrid Models are created using Aspen AI Model Builder™, a SaaS application running in the cloud. This application enables you to define and collect data from different sources (plant data, simulation data, Aspen Multi-Case™, etc.), aggregate data, model data, apply insights and build the model to be deployed to different products: Aspen HYSYS, Aspen Plus, Aspen PIMS-AO and Aspen Unified for PIMS and GDOT.

In the case of First Principles-driven models, all these steps are available within Aspen Plus and Aspen HYSYS.

### 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 and later. In Aspen HYSYS and Aspen Plus V12 and later, you 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.



## Which products and versions support Aspen Hybrid Models?

- AI-driven and Reduced Order Hybrid Models can be deployed directly in both Aspen HYSYS and Aspen Plus V12 and later, and used in digital twin applications through Aspen OnLine.
- Reduced Order Models are available for Aspen Unified, V12.1 and later to update nonlinear planning models in PIMS and for dynamic optimization in GDOT.
- First Principles-driven Hybrid Models are available starting with Aspen Plus and Aspen HYSYS V12.1.
- It is also possible to deploy models in Aspen HYSYS and Aspen Plus V10 and V11, and in PIMS-AO V12 and later, following some additional steps.

## Aspen AI Model Builder

### What are the applications of Hybrid Model created with Aspen AI Model Builder?

The workflows available to deploy models created in Aspen AI Model Builder are:

- AI-driven Hybrid Models deployed to engineering
- Reduced Order Hybrid Models deployed to engineering
- Reduced Order Hybrid Models for planning
- Reduced Order Hybrid Models for GDOT

AI-driven Hybrid Models can be deployed to Aspen HYSYS and Aspen Plus as a sensor or as equipment (either a single piece of equipment or an entire flowsheet). A Reduced Order Hybrid Model can also be deployed to Aspen HYSYS and Aspen Plus as sensors or equipment. Reduced Order for planning will create a nonlinear planning submodel to be used in the Aspen PIMS-AO or Aspen Unified PIMS refinery model.

Reduced Order for GDOT will create a fit-for-purpose model that combines the power of machine learning with the accuracy of first principles models to incorporate complex reactor units within the scope of online optimization through Aspen Unified.



## Do I need Aspen Multi-Case to create a model in Aspen 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 continually looking for secure ways to improve the interpretability of the model. After models are created, Aspen 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.

You 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 you 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 in running 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 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, you 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 you quickly compare the results without having to go through the complete design of experiments.

### **How is the security addressed with uploading data to the cloud?**

Everyone has a unique login, where nothing can be shared between individuals. 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 you 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 anyone, including... planner and control engineer.

### **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.

### **How do you test the accuracy of the results in locations 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 AI Model Builder is a cloud-based product deployed in the Aspen Cloud, which means that it does not need any local installation.

Aspen Plus, Aspen HYSYS and Aspen Multi-Case are desktop tools, like the rest of the Engineering suite. You can run Aspen Multi-Case locally on your own computer or in a high-performance server shared by many people. Similar to the Engineering products, Aspen PIMS and Aspen GDOT are also desktop tools, while Aspen Unified is a web-based application.

### **What is the difference between sensor and equipment models?**

An inferential sensor, virtual sensor or just “sensor” is deployed within Aspen HYSYS or Aspen Plus to predict properties inside your design or operations model. This sensor 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 variables such as temperature, pressure or composition are unknown.

Aspen Hybrid Model equipment refers to a piece of equipment such as a reactor or a membrane. It can also refer to a section of a flowsheet or a complete flowsheet that can be used for sitewide 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.

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

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