Frequently Asked Questions About Aspen Hybrid Models™

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Building on AspenTech's 40-plus years of chemical and energy processing expertise, Aspen Hybrid Models combine the domain experience of engineering first principles and the intelligence of Industrial AI to create accurate high-fidelity models faster without requiring significant expertise. This next-generation solution lowers the total cost of ownership and reduces the time to value of utilizing models across the asset lifecycle.

This document answers commonly asked questions about Aspen Hybrid Models.

Q: Why are Aspen Hybrid Models important?

A: Providing broad access to more comprehensive and more accurate models, across all the phases of the asset lifecycle, is a crucial step in understanding and predicting how specific processes will behave safely and efficiently. As assets and their systems have increased in complexity, higher predictivity of models has become essential to design, operations and maintenance. With Aspen Hybrid Models, users can model processes and assets that cannot easily be modeled with first principles alone. You get the accuracy of empirical models, the strength of first-principles models, leveraging the power of Industrial AI, along with 40-plus years of domain expertise, to create a more predictive model.

Q: At a high level, how do Aspen Hybrid Models work?

A: The technology democratizes the application of Industrial AI to optimally design, operate and maintain assets—online and via edge—modeling processes and assets which cannot easily be modeled with first principles alone.

Machine learning is used to create the model, leveraging process simulation (with Aspen HYSYS® or Aspen Plus®) or plant operations data, while using domain knowledge, including first principles and engineering constraints to build an enriched model. This can be done without requiring significant modeling or AI expertise.

Q: What benefits can engineering firms expect by adopting Aspen Hybrid Models?

A: Organizations are able to create a better-performing model, perform more frequent analysis and continuously achieve greater results. Aspen Hybrid Models provide an end-to-end workflow to create and sustain more accurate, longer-term models.

Key benefits include:

- Represent real plant behavior with models created from operational data and applying first-principles constraints
- Improve controller performance and operational stability by supplying high fidelity, nonlinear models for advanced process control
- Enable faster, more accurate decision-making in engineering and operations to recapture value
- Easily incorporate complex process units to the scope for closed loop optimization

In addition, 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. Aspen Hybrid Models enable 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.

Q: Why do first principles matter?

A: First principles:

- Avoid unrealistic results due to plant-model mismatch, non-physical relationships apparent in data and noisy derivatives
- Provide additional structure and insight, enabling accurate models with less empirical data
- Establish guardrails for extrapolating into regions with no data
- Improve user acceptance when deploying in operations
- Solve use cases which could not be addressed without constraints

First-principles models are the modeling systems that have been created with over four decades of chemical engineering know how—and they play a fundamental role in the scope, breadth, safety and sustainability of the industry today.

Q: What benefits can Aspen Hybrid Models provide in planning?

A: Planning model accuracy can be increased by over 97%, 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.

Q: How do Aspen Hybrid Models assist control and optimization?

A: High-fidelity unit optimization models enable model alliance between process engineering, planning and process control. Nonlinear optimization with these models improves accuracy of the optimization, leading to increased profits and reduced margin leakage.

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

A: With a focus on managing constraints, we leverage our domain knowledge to ensure that the 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 DMC3™, Aspen GDOT™, 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

Q: What are the main applications for Aspen Hybrid Models?

A: 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 models for planning and advanced process control

Fast asset-wide models

- Integrated upstream and midstream facilities
- Integrated oil-to-chemicals
- Sitewide optimization
- Sitewide 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

Models for real equipment performance

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

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

A:

- Oil and gas separation
- Hydrate formation and inhibition
- Property sensors (pH, Reynolds)
- LNG plant
- Natural gas dehydration
- Sales gas dew point
- Compressor trains
- CO_2 freeze temperature

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

A:

- 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

Q: What are the primary applications in bulk chemicals?

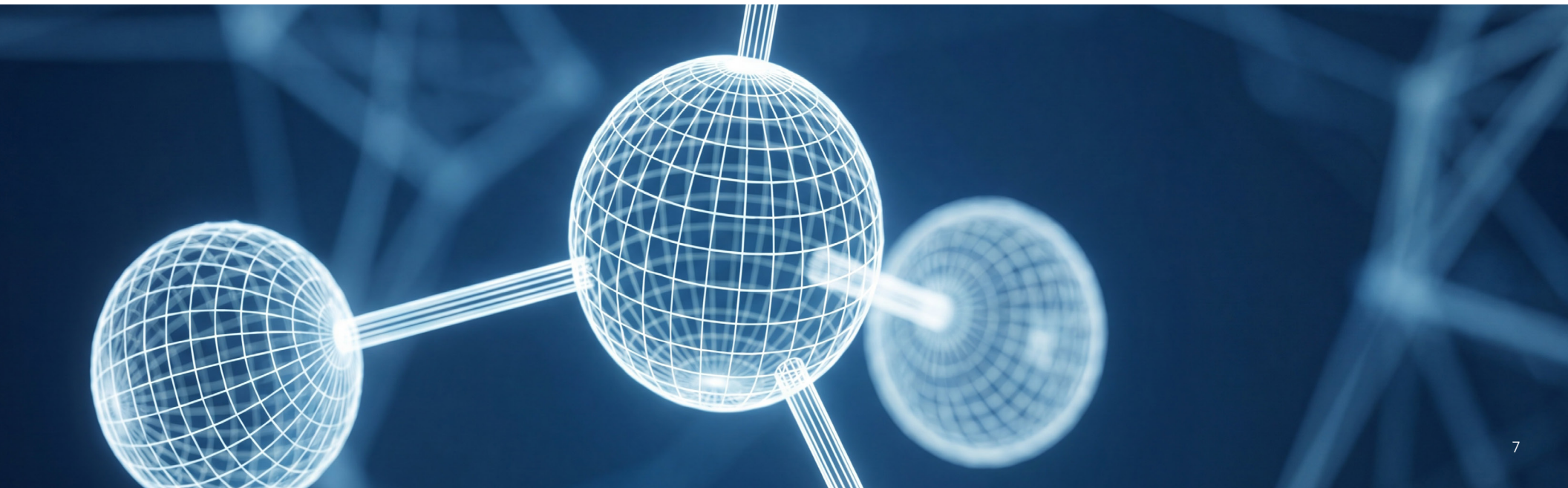
A:

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

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

A:

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



Types of Aspen Hybrid Models

Q: What are the different types of Aspen Hybrid Models?

A:

- AI-driven Hybrid Models
- Reduced-order Hybrid Models
- First-principles-driven Hybrid Models

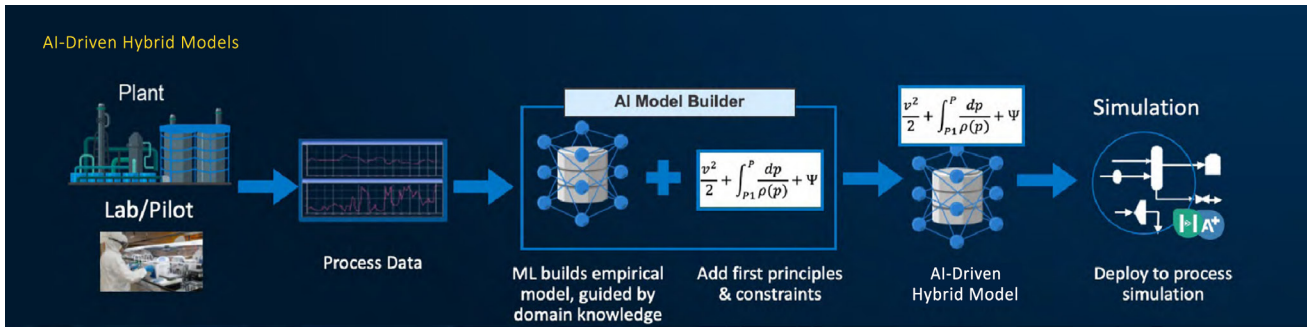
Q: What is an AI-driven Hybrid Model?

A: 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 that 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

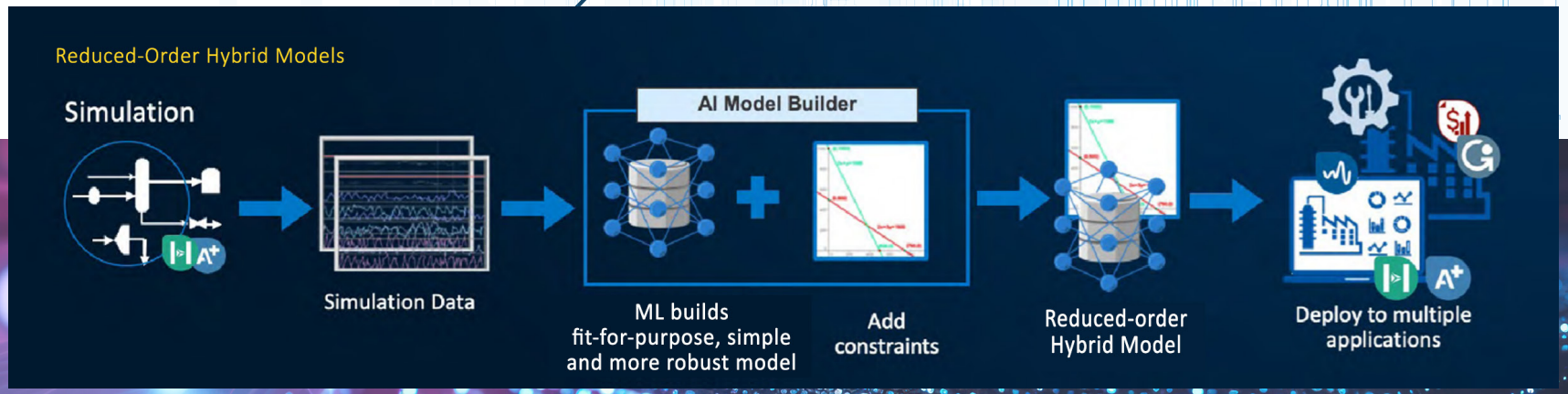


Q: What is a reduced-order Hybrid Model?

A: 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

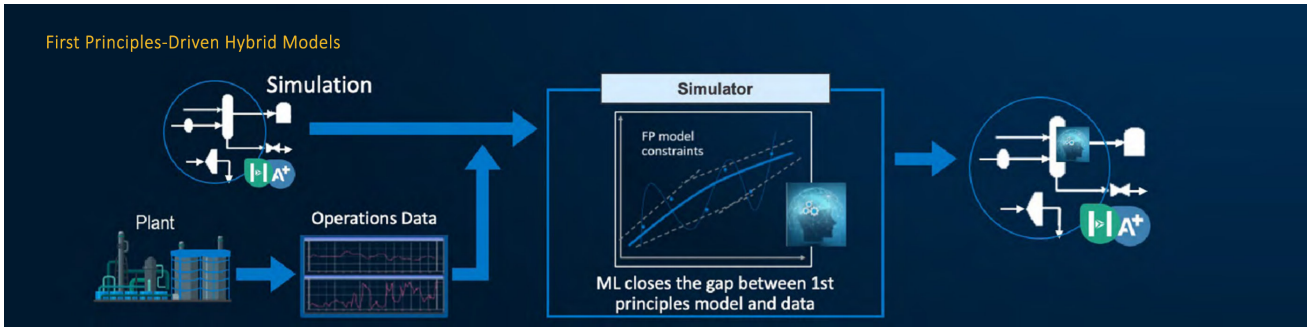


Q: What is a first-principles-driven Hybrid Model?

A: With the first-principles-driven 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



Q: Can the different types of Aspen Hybrid Models work together?

A: 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.

Q: What are the different steps to creating a Hybrid Model?

A: AI-driven and reduced-order Hybrid Models are created using Aspen AI Model Builder™. 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.

Q: Can you deploy an Aspen Hybrid Model online?

A: 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 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).

Q: Which products and versions support Aspen Hybrid Models?

A:

- 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 Hybrid Models are available for Aspen Unified, V12.1 and later to update nonlinear planning models in PIMS, for dynamic optimization in Aspen GDOT and advanced process control in Aspen DMC3.
- 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, with additional steps.

Aspen AI Model Builder

Q: What are the applications of Hybrid Models created with Aspen AI Model Builder?

A: 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 Aspen GDOT
- Reduced-order Hybrid Models for Aspen DMC3

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 Hybrid Models for planning will create a nonlinear planning submodel to be used in the Aspen PIMS-AO or Aspen Unified PIMS refinery model.

Reduced order Hybrid Models for Aspen 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. Reduced order Hybrid Models for Aspen DMC3 will create a fit-for-purpose model that combines the power of machine learning with the accuracy of first-principles models to incorporate into advanced process control.

Q: How do I deploy Aspen AI Model Builder?

A: Aspen AI Model Builder can be deployed on your desktop like any other AspenTech Performance Engineering software.

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

A: 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.

Q: Are there features that provide confidence in the model's accuracy?
A: 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.

Q: How do Aspen Hybrid Models and Aspen Multi-Case handle convergence issues?
A: 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 created within the reduced-order Model, this will not present a convergence issue.

Q: What is an advantage of not displaying the data used to create Aspen Hybrid Models?
A: 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 models are created and used.

Q: Are services required to create and implement Aspen Hybrid Models?
A: Aspen AI Model Builder was designed so you can build the models yourself. Data science expertise is not required to apply AI in the process industry or 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 planners and control engineers.

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

A: Our guidance is to build models 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 this data with simulation data to cover regions where plant data is sparse.

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

A: Since Hybrid Models are 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 receive a warning that the model has solved outside of the training bounds.

General

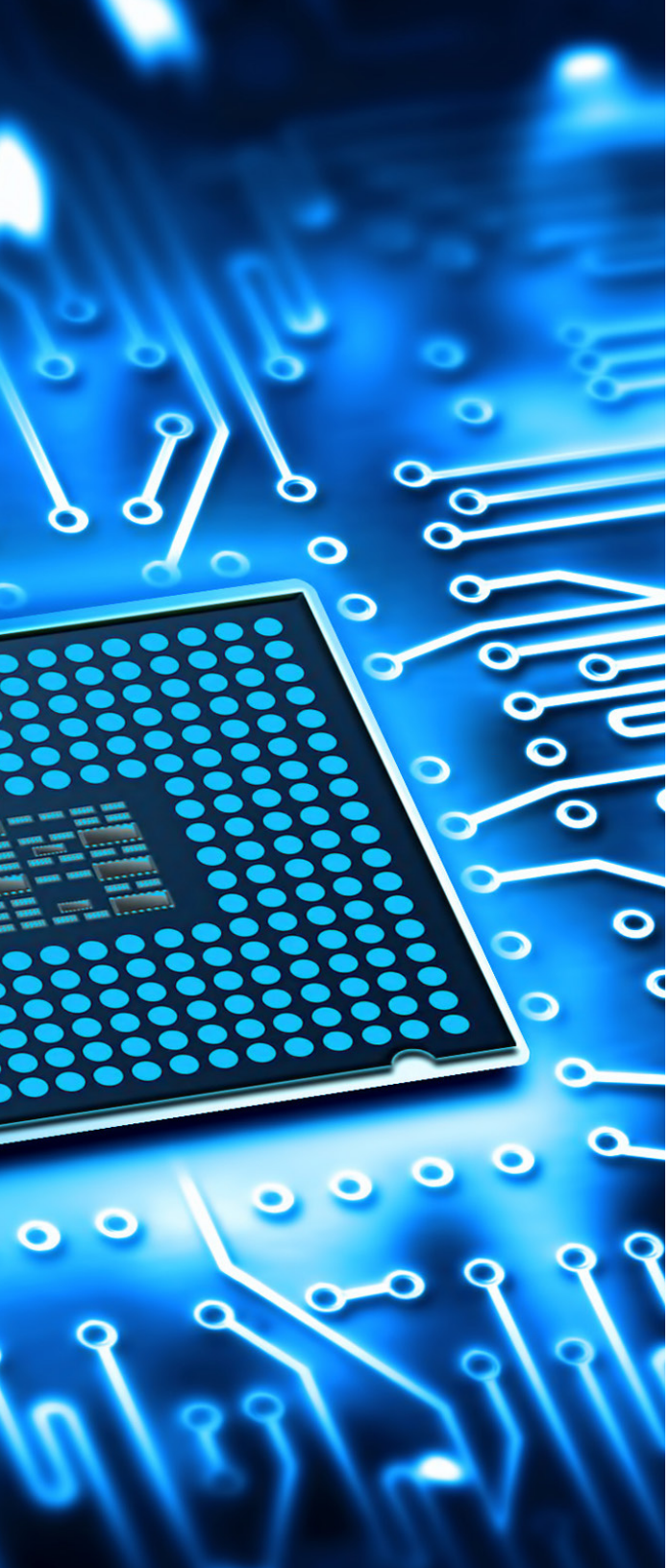
Q: Can I install these tools on a local laptop or do they need to be on a server?

A: Aspen AI Model Builder can be installed on any user desktops. 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 other users. Similar to the Engineering products, Aspen PIMS and Aspen GDOT are also desktop tools, while Aspen Unified is a web-based application.

Q: What is the difference between sensor and equipment models?

A: 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 Models equipment refers to a piece of equipment such as a reactor or 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.



Resources

Q: Who is using this technology?
A: Organizations across the world are using Aspen Hybrid Models. Here are a few examples of how companies benefit from these capabilities.

- **Mitsubishi Chemical Uses Aspen Hybrid Models to Detect and Avoid Product Quality Issues**
- **Petro Rabigh Uses Aspen Hybrid Models™ to Improve Margin and Reduce Operational Risk**
- **Aspen Hybrid Models™ - A Closer Look**

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 Hybrid Models webinars:

- **Unleash the Power of Hybrid Modeling for Process Design and Optimization Featuring Dow**
- **Drive Production Optimization To Achieve Margin and Energy Efficiency**

Q: Are there any how-to videos available?
A: Several how-to videos are available on the **AspenTech Support Site.**

Didn't see your question answered here? Visit our Aspen Hybrid Models page or **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.

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