# Hybrid Models in Chemicals: Leveraging Industrial AI to Overcome Operational Challenges

**Webinar Q&A**

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During the November 5, 2020 **webinar "Hybrid Models in Chemicals: Leveraging Industrial AI to Overcome Operational Challenges"** several participants asked technical questions about Aspen Hybrid Models™ in Aspen Plus®. AspenTech experts have consolidated the questions and provided answers below.

Additional questions should be directed to **AspenTech Support**

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# Importing Data to Create Aspen Hybrid Models

**Q: What sources can be used to import the data for creating a hybrid model?**

A: You can import data from any source as long as it is in the format supported by Aspen AI Model Builder™ (simulations, operations, lab, pilot plant, etc.). In a reduced order hybrid model (ROM) you can import simulation data generated by Aspen Multi-Case™. All the workflows accommodate upload data in .csv format from any source.

**Q: How much time does it take from the first principles model to building the hybrid models?**

A: Build time varies based on the complexity of your problem, how quickly each individual case runs and the hardware available. With Aspen Multi-Case you can run many cases in parallel and the speed will depend on how many cores you have available for computing. Usually, a ROM model will need at least 1000 simulation cases, which could take minutes or hours to run on a multi-core machine. Once the ROM model is built and deployed into an Aspen Plus or Aspen HYSYS® case it will run very quickly (30 seconds).

**Q: What does Aspen Multi-Case do?**

A: Aspen Multi-Case is one of the newest products in aspenONE® V12. It is a smart design of experiments technique that uses parallel computing to run hundreds of simulation cases concurrently, significantly faster as compared to conventional case study features. It runs cases in parallel on multi-core computers. Aspen Multi-Case can also perform parallel case studies across two or more models with different topologies, allowing comparison of different designs.

**Q: Is there any data assessment methodology to ensure that we have enough suitable data to develop a Hybrid Model?**

Aspen Multi-Case uses a smart sampling technique to ensure good representation of the variable space. In addition, AI Model Builder has some heuristics to require a certain minimum amount of data.

**Q: How does this model work on dimensionless scales where fundamentals are not correctly produced during simulation?**

A: If the dataset you upload contains tags which do not have a physical type, we will only be able to build a pure machine learning model. In order to perform first principle augmentation, you will need to provide more information on individual variable types and how they map to corresponding streams.

# Creating Aspen Hybrid Models

**Q: Which kind of machine learning algorithm is the model based on?**
A: The different workflows (reduced order models versus AI-driven) use different algorithms which were found to work best for each class of problems. For ROM models, our R&D team found the polynomial approach is very good for speed and reliability. Note that feature selection is largely automated: the system tries different options and eliminates the features that do not improve the models.

**Q: Can we specify the specific machine learning algorithm in case that we found a low predictability problem?**
A: The current model lets you optionally apply high order (third order) polynomial terms which also activate additional cross terms. We are planning to improve this by adding a wider range of algorithm options to provide more alternatives.

**Q: Does AspenTech allow building neural network models with varying layers and activation functions?**
A: Not in the AI Model Builder. We will keep researching and implementing additional algorithms and will consider such improvements in the future.

**Q: What AI models are being used by the hybrid models? Can we specify or experiment with different models?**
A: Currently we are using a combination of LassoCV and Reluctant Modeling. In the future, we are looking to introduce more model building techniques and allow the user to experiment with different options.

# Data Cleaning and Improving the Model

**Q: Can users see inside the AI model and make modifications?**
A: Aspen AI Model Builder has features that help interpret the results of the model. Users have some level of control over the algorithms in different workflows, for instance, increasing the order of polynomial regressions for reduced order models.

**Q: What data analysis tools are provided to review the results?**
A: During the validate model step, we provide information on accuracy (R2) and predictability (Q2) for each dependent variable within the model. In the model details, you will also be able to see information on the mean average error for each dependent variable. You can view parity plots (predicted vs data) for all variables. You can also raise "contribution" plots to see how strongly dependent variables are influenced by independent variables.

**Q: For AI-driven hybrid models, are the physical laws of conservation and thermodynamics checked? What if the plant data selected does not make sense?**
A: During the model building phase, the AI Model Builder checks mass balance and imposes penalties to drive the solution towards mass balance closure. After the model has been created and validated, we can export and deploy the model to Aspen Plus. At this stage, we will use the hybrid model in the same way we would use any other unit operation. The material streams going in and out of the hybrid model will be checked to ensure we are not violating any thermodynamic laws. It is also possible to clean data to remove data that we know is not right. The system also checks the limits of all independent variables to ensure they are within the training range of the original data set, and dependent variables are checked to ensure they are within the predicted ranges of the original training set. The system reports warnings when variables are out of range.

**Q: How do you combine analytical data that is not continuous as process variable?**
A: If you are using a dataset with variables that are sampled at different intervals, it is best to try and align them first outside of the AI Model Builder before importing to avoid gaps in the datasets.

**Q: Are internal variables generated based on phenomena we add, like mass transfer in membrane?**
A: When you select a specific phenomenon (e.g. mass transfer), the AI Model Builder will automatically calculate additional variables based on the dataset. We have a library of equations within the application that will be included based on the dataset and user specifications.

# Data Security

**Q: How is the security addressed considering we may update sensible plant data?**
A: 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.

# Deploying Aspen Hybrid Models

**Q: How much time does it take to run a hybrid model?**
A: On the deployment side, hybrid models run in a few seconds. It depends on the degree on non-linearity of the model. For example, if you have a larger number of terms or variables, the model might take longer to run.

**Q: Can I use this in previous versions of Aspen Plus?**
A: Aspen Hybrid Models can be used in Aspen Plus V12. You can also export models for use in Aspen Plus V10 or Aspen Plus V11.

**Q: Will the model still go through your cloud while running?**
A: No, Aspen AI Model Builder is a SaaS application used only to create the model. Once deployed to Aspen HYSYS or Aspen Plus, you will run Aspen HYSYS or Aspen Plus as you normally do through either a local install or a cloud installation.

**Q: Can the Hybrid model be deployed outside the Aspen environment? For example, in MS Excel?**
A: Aspen Hybrid Models are designed specifically to be recognized and utilized seamlessly into AspenTech products such as Aspen Plus, Aspen HYSYS and Aspen PIMS™.

**Q: Will there be any convergence issues if there are lot of recycles while working with site-wide hybrid models?**
A: If the model is well structured, there should not be any trouble 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. If the recycle loop is created within the reduced order model, it will not present a convergence issue. If the recycle is outside the reduced order model, when you deploy into Aspen Plus or HYSYS, the model uses the same convergence strategy already built in the simulator.

**Q: Can I import my own ML model as a 'user defined unit' to the Aspen simulation model?**
A: Aspen Plus provides two unit operation interfaces: USER2 (sequential) and USER3 (equation-based). These are FORTRAN APIs but they can easily be configured to call models compiled in other languages such as C# using a 'wrapper.'

# Installation

**Q: Can I install these tools on a local machine or do they need to be on a server?**
A: 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 — it does not need local installation.

# Usability of Hybrid Models

**Q: Does the model indicate if it is in the "extrapolation" area?**
A: Once you run this model in Aspen HYSYS or Aspen Plus, you will get warnings if you run it outside the original training range.

**Q: How do you test the accuracy of the results in areas without plant data?**
A: 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 will issue a warning that it has solved outside of the training bounds.

**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 a model using a 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.

**Q: When doing optimization, is there a way to guarantee that the optimum point of a reduced order model is in the range of the optimum obtained when you use the first principal model?**
A: Parity plots for accuracy and predictability will show how well the model matches specific data points. Once the model is deployed, it could also be validated with sensitivity studies to compare the first principles model with the reduced order hybrid model.

**Q: Can we use this approach to model phenomena that take place inside a reactor?**
A: If you have plant data or lab data you can build a model which considers the real plant experience. This could address phenomenon such as non-ideal mixing which first principles models like RCSTR do not consider.

We are also working on first principles-driven hybrid models which brings a neural net inside Aspen Plus to predict phenomenon such as rate expressions: the model tunes itself using reinforcement learning to train the neural network to match measured data.

**Q: Is there an option to model the residuals to create parallel hybrid models?**
A: We do not currently offer any features for modeling hybrid model residuals.

**Q: Can this AI model builder be used to create inferentials for APC applications?**
A: We do not currently offer any direct integration points between Aspen Hybrid Models and APC.

**Q: Is it possible to export one of these models into a process model for a DMC3 controller?**
A:  We have developed a specific workflow to deploy reduced order hybrid models from Aspen HYSYS refining models to update Aspen PIMS planning models. We eventually intend to use these models to seed Aspen DMC3™ and GDOT™ models to get nonlinear gains from the hybrid model.

# General Questions

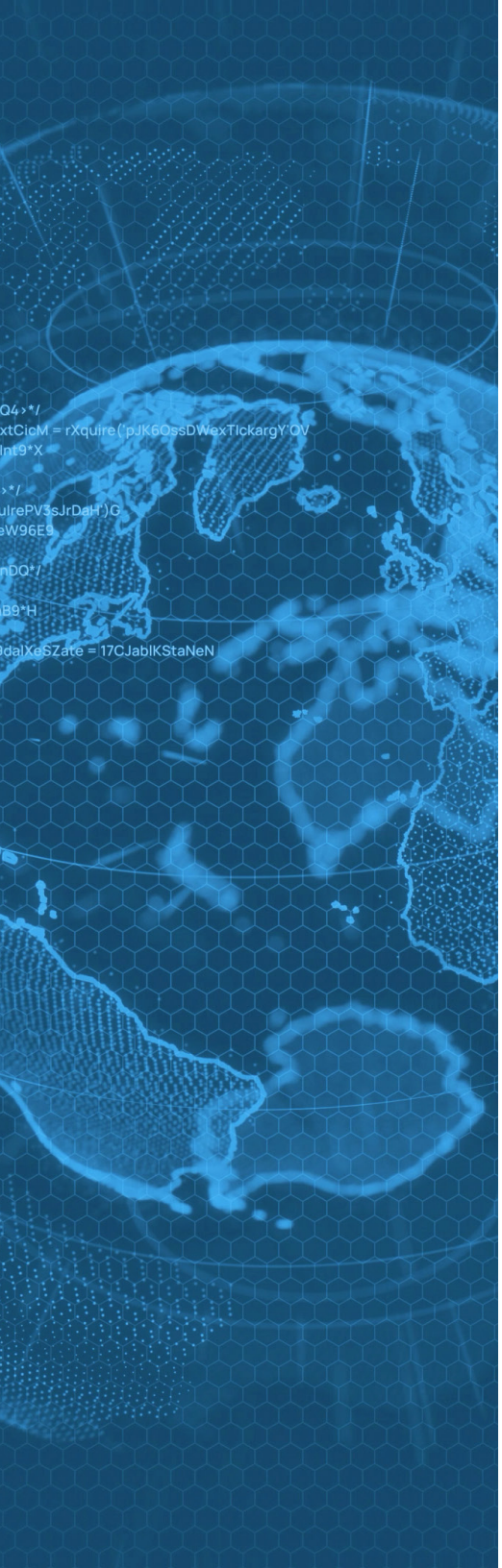
**Q: How does the model handle dynamic effects in the plant data?**
A: The AI Model Builder is currently designed for steady-state processes. We are considering batch and dynamic applications in the future. We have several research projects in this area with some promising successes. For data generation, Aspen Multi-Case can generate data from process simulations that contain batch units.

**Q: Is Equation Oriented Modeling supported?**
A: Support for EO simulations will be considered in the future. As a data source, it is possible to use Aspen Simulation Workbook's scenario feature to generate case studies with an Aspen Plus or HYSYS EO model. These can be saved into .csv files and imported into AI Model Builder.

**Q: Will this include dynamic reconciliation against plant data?**
There are many use cases in industry to address time-dependent phenomenon and we have had some promising successes with research projects to consider these improvements in the future. As part of V12, our colleagues in the APC team have delivered deep neural net algorithms as part of Aspen DMC3.

**Q: Can this application extend to thermodynamic models, e.g. for complex chemistry?**
When a user has enough data, it is recommended to fit binary parameters with data regression in Aspen Plus, which is designed specifically for this class of problems.

First principles-driven hybrid models may offer additional flexibility to use AI to calibrate and extend an existing Aspen Plus or HYSYS model.



# Aspen Hybrid Models Applications

**Q: What other types of process can these modeling systems simulate?**

A: You can apply reduced order hybrid models to a wide variety of processes since they are based off existing Aspen HYSYS or Aspen Plus models. If you are looking to build a more accurate model for a specific asset, an AI-driven hybrid model may be a good choice. AI-driven hybrid models can generate models from a wide variety of sources including plant data, lab data, field data or simulation data.

# Aspen Hybrid Models Licensing

**Q: How is Aspen Hybrid Models licensed?**

A: For details on licensing, please contact your sales representative or the key contacts referenced below.

# Contact Us

**Q: How can I contact the webinar presenters?**

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**Q: What if I have more technical questions?**

Please direct any additional questions to AspenTech Support: **esupport@aspenetch.com**

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