

# Adding automation and data analysis to process simulators with MATLAB

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  - UNC Chapel Hill



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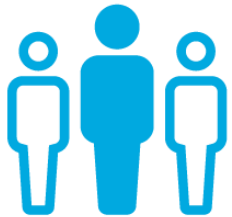
**North America**  
United States

**Europe**

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France  
Germany  
Ireland  
Italy  
Netherlands  
Spain  
Sweden  
Switzerland  
UK

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Korea



**5500+ staff**  
in 33 offices around  
the world



**\$1+ billion**  
in 2020 revenues



**5 million+**  
users in over  
185 countries



**100,000+**  
businesses, governments,  
and universities



**Privately held**  
founded 1984



is a **Leader** in the 2021 Gartner Magic Quadrant for Data Science and Machine Learning Platforms for the Second Year in a Row

Figure 1: Magic Quadrant for Data Science and Machine Learning Platforms



Source: Gartner (March 2021)

Gartner Magic Quadrant for Data Science and Machine Learning Platforms, Peter Krensky, Carlie Idoine, Erick Brethenoux, Pieter den Hamer, Farhan Choudhary, Afraz Jaffri, Shubhangi Vashisth, 1st March 2021.

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# The manufacturing industry recognizes MathWorks as the top choice for data science and machine learning



is the highest ranked Customers' Choice for the **Manufacturing Industry** for Data Science and Machine Learning Platforms based on number of reviews and overall rating.



Figure 8. Gartner Peer Insights “Voice of the Customer” Data Science and Machine Learning Platforms Manufacturing Industry



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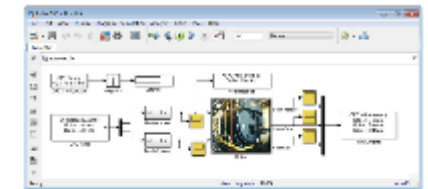
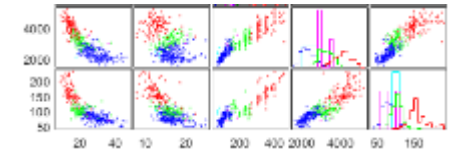
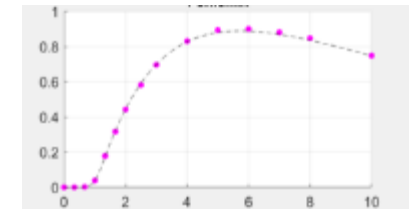
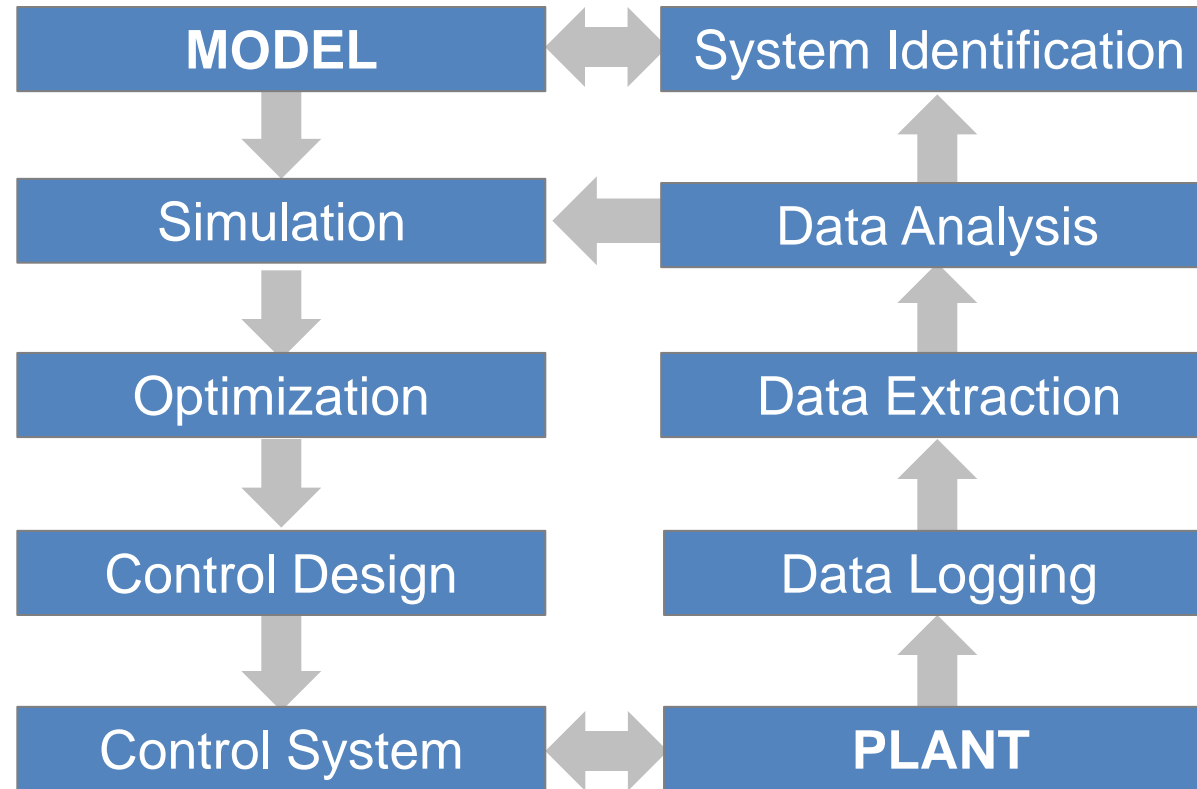
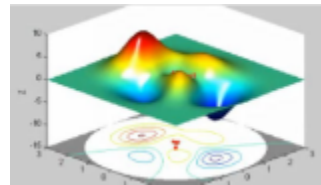
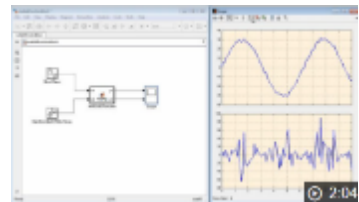
# IEEE Top Programming Languages 2020

Rank	Language	Type	Score
1	Python▼	🌐 🖥️ ⚙️	100.0
2	Java▼	🌐 📱 🖥️	95.3
3	C▼	📱 🖥️ ⚙️	94.6
4	C++▼	📱 🖥️ ⚙️	87.0
5	JavaScript▼	🌐	79.5
6	R▼	🖥️	78.6
7	Arduino▼	⚙️	73.2
8	Go▼	🌐 🖥️	73.1
9	Swift▼	📱 🖥️	70.5
10	Matlab▼	🖥️	68.4

# Process Engineering Workflow

Process engineering leverages data and modeling to design and continuously improve plants.

$$\frac{d^2 x}{dt^2} - \mu(1 - x^2) \frac{dx}{dt} + x = 0$$



MathWorks provides a comprehensive suite of software tools to support this workflow.

# Use cases for integrating MATLAB with process simulators

**P**  $K_p e(t)$

**I**  $K_i \int e(\tau) d\tau$

**D**  $K_d \frac{de(t)}{dt}$

## Control Strategy

$r_A = k C_A C_B$

Equations (4.56) and (4.58)

$\frac{dC_A}{dt} = -k C_A C_B - \frac{F_0}{V} C_A$

$\frac{dC_B}{dt} = k C_A C_B - \frac{F_0}{V} C_B$

$V = V_0 + v_0 t$

## Custom Unit Operations

Compression System  
 $[Y_1, v, Y_2]$   
 $[Y_1, v, Y_2]$

K-100  
 E-100  
 K-102

## Scenario modeling

feasible region

non-dominated solutions

## Multi-objective optimization

$x_1, x_2, x_3$

Model  $f(x)$

$y_1, y_2$

Reliability = 26.40.04

## Sensitivity analysis

## Dynamic optimization

## Automating repetitive tasks

Model

Covariance matrix

Data reconciliation

## Pre-processing data

Hidden layer

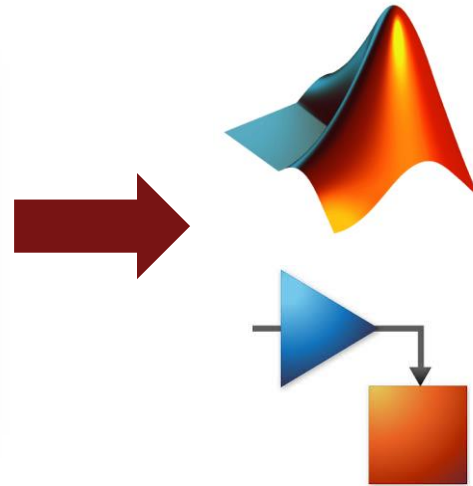
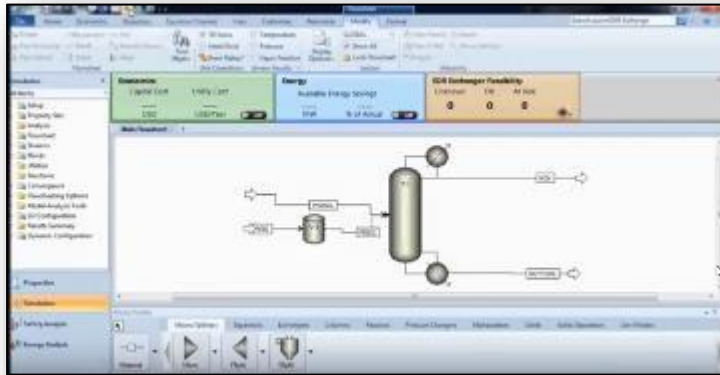
## Machine Learning



# Connecting to process simulators

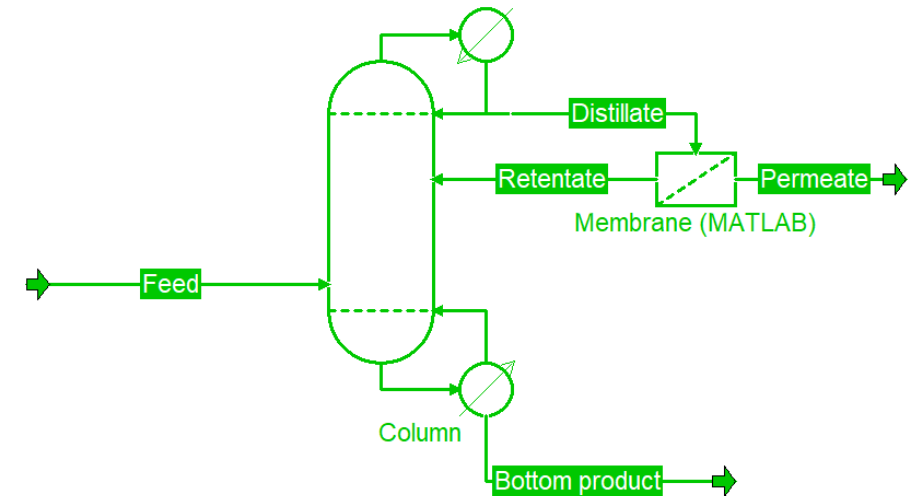
## Calling simulators from MATLAB

- Using ActiveX automation server
- Using native integration



## Embedding MATLAB in simulators

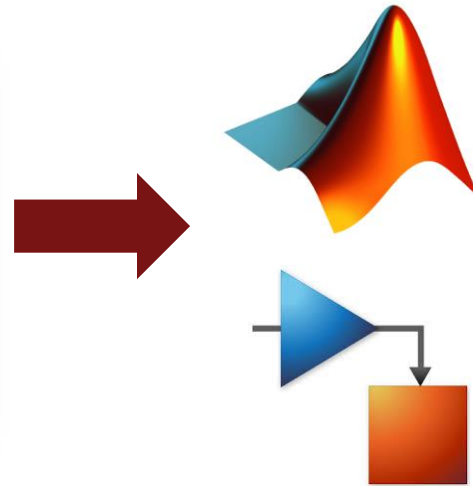
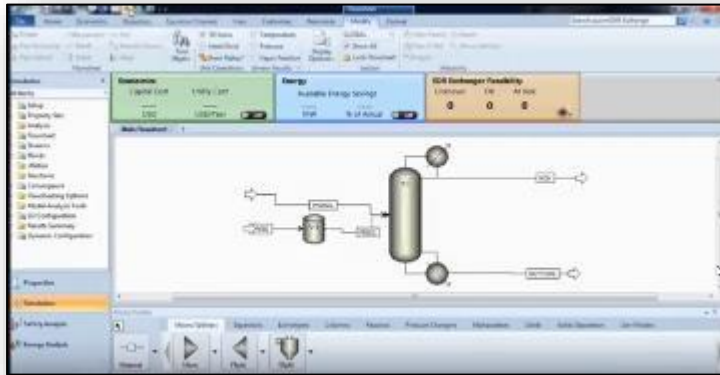
- Using CAPE-OPEN
- Using HYSYS extension container



# Connecting to process simulators

## Calling simulators from MATLAB

- Using ActiveX automation server

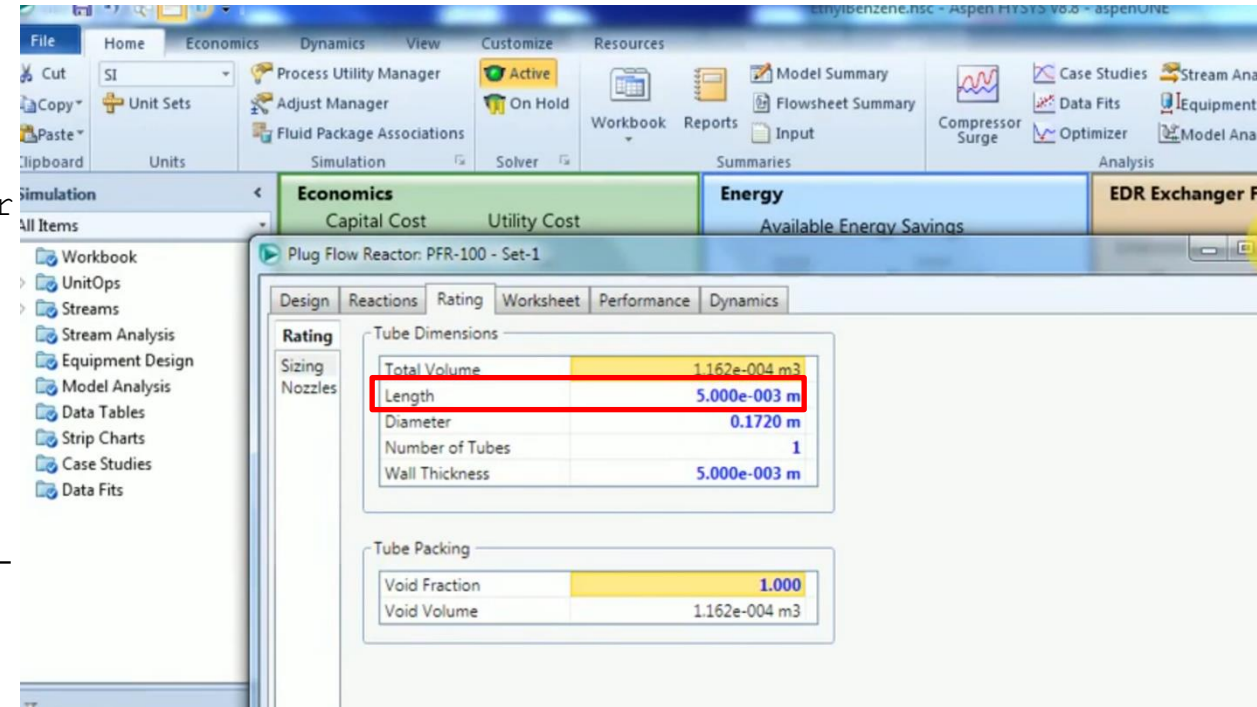


# Alter HYSYS flowsheet values programmatically within MATLAB through COM automation server

```

a = actxserver('Hysys.Application'); %opening the
application
SimCase =
a.SimulationCases.Open([cd, '\EthylBenzene.hsc']); % your
filename here.hsc%
SimCase.visible = true;
% Find the address of a stream or variable
b=get(a.activeDocument);
c=get(b.Flowsheet);
d=get(c.Operations);
d.Names
h=get(a.activeDocument.Flowsheet.Operations,'Item','PFR-
100');
i=get(h)
%Change Tube length of PFR
h.TubeLengthValue=0.005;

```



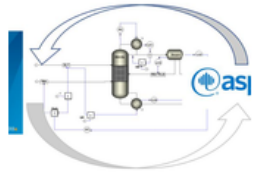
# Connecting MATLAB to Aspen Plus



Products Solutions Academia Support **Community** Events

## File Exchange

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## Aspen Plus - Matlab Link

version 1.1.0 (1.8 KB) by Afabrild

This file outline the Aspen Plus and Matlab connection through COM Technology.

Overview

Functions

Simulation of chemical process is essential to develop sustainable designs. Nowadays, with the competitiveness in the markets, it demands the optimal operation of any chemical plant. In the new designs of chemical processes, design optimization is mandatory.

Matlab is a program widely used and accepted by the academic community. Academics daily load codes with advanced numerical methods of great application for engineering. Advanced optimization methods must be taken into account to apply them in the optimal design of chemical processes. Therefore, the connection between chemical process simulation programs (Aspen Plus, Hysys, Pro II, etc.) and tools such as Matlab are very useful.

Also, several people have written me to the email requesting an example. See post in ResearchGate:  
[https://www.researchgate.net/post/How\\_can\\_I\\_integrate\\_Aspen\\_Plus\\_and\\_Matlab\\_for\\_optimization\\_propose](https://www.researchgate.net/post/How_can_I_integrate_Aspen_Plus_and_Matlab_for_optimization_propose)

I present an example of connection between Aspen Plus V.10.0 and Matlab. The simulation corresponds to a reactive distillation column. As an application of the connection, a sensitivity analysis is done using Matlab (for loop).

Its only necessary to place the two files in a folder and run the AspenPlus\_Matlab.m

Simulation file (Aspen Plus V.10.0) in: <https://drive.google.com/open?id=1oSqqMj11h3NJIHPIhzCeok9baaH4PHnC>

Requires Aspen Plus V.10.0 software

Google 'Aspen Plus MATLAB'

# Flowsheet structure optimization with MATLAB and HYSYS

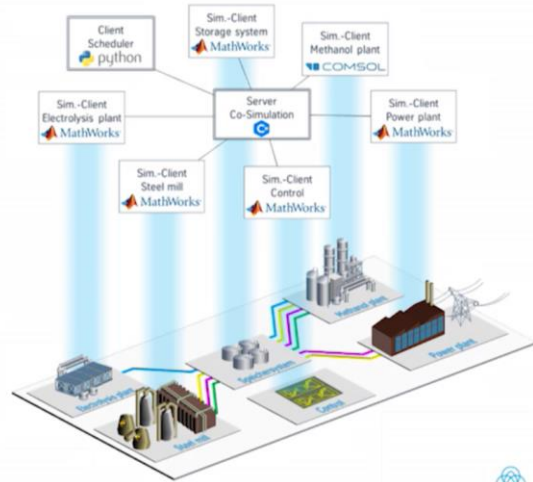
## Integration of Modular Process Simulators under the Generalized Disjunctive Programming Framework for the Structural Flowsheet Optimization

Miguel A. Navarro-Amorós , Rubén Ruiz-Femenia , José A. Caballero

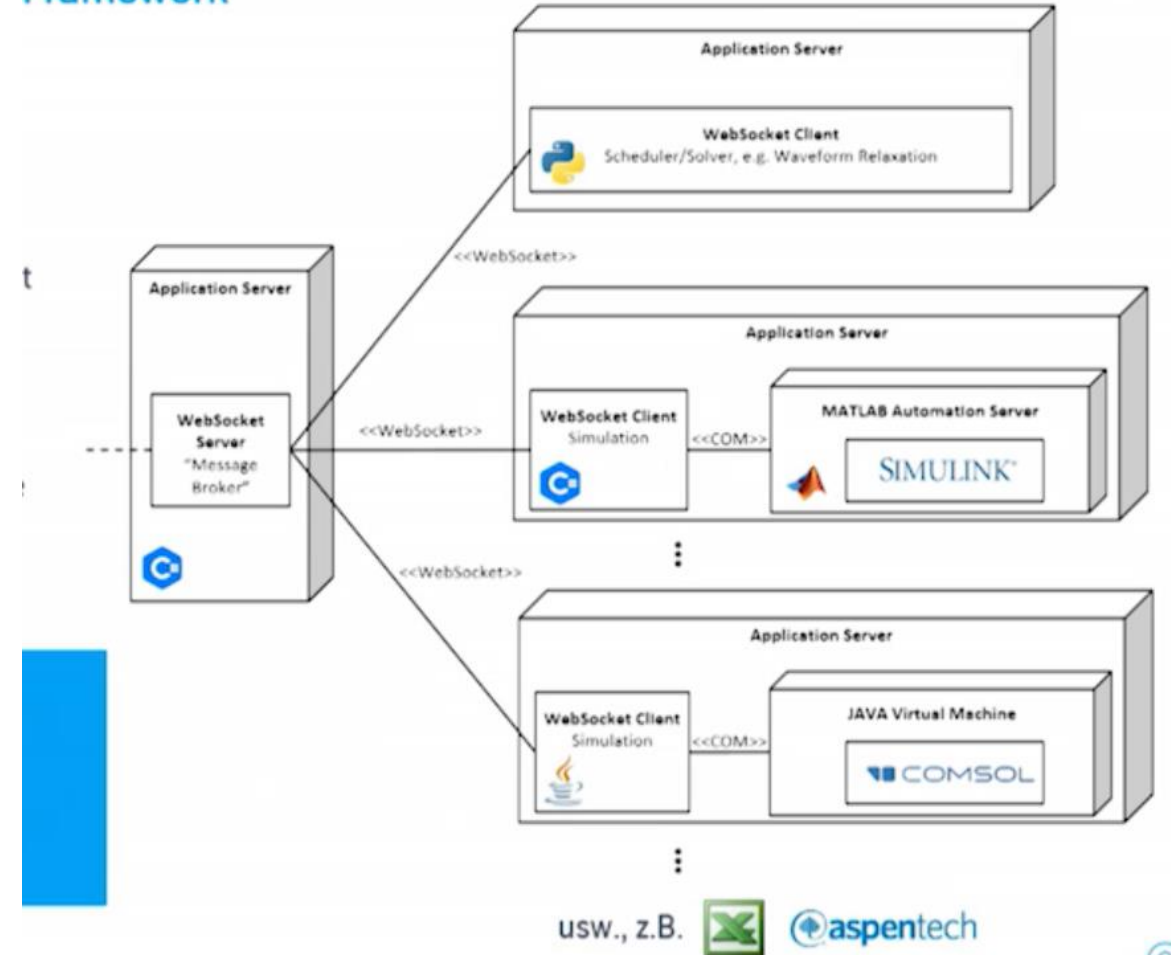
# Thyssenkrupp co-simulates MATLAB with Aspen Plus and COMSOL to model CCU plant

## Das Carbon2Chem® Co-Simulations-Framework

- Server-Client Architektur
- Verschlüsselte webbasierte Kommunikation (WebSocket) über definiertes Interface
- Lösungsverfahren der Gesamtsimulation in Client „Scheduler“ implementiert
- Modelle und deren lokale Solver in speziellen Simulationsprogrammen implementiert
- Integration von Simulatoren über konfigurierbare WebSocket-Clients



## Framework



# Dow saves hundreds of engineer hours by integrating MATLAB with Aspen Plus for Process Optimization

## ACHIEVING HIGH THROUGHPUT MODELING

- MATLAB is a powerful software for developing models and performing optimization
- ### NEW COLUMN DESIGN AND OPTIMIZATION: MAN VS MACHINE

- MATLAB and Aspen Plus were used to evaluate the design of a new column. The design was evaluated by both a human and a machine.

### A VERY IMPACTFUL CAPABILITY!

- Using the combination of Aspen and MATLAB in this application presents a tremendous new capability that will be leveraged into the future:

- Case 1:** Conventional design
  - Variables to adjust: 5
  - Results comparison: 5

- Better product consistency** – battery of operating conditions can be modeled to test against existing processes
- More robust operation** – test controls/develop control schemes for processes. Demonstrate if improvements will be robust enough to provide the needed reliability/stability

- MATLAB can now provide results
- Case 2:** Column with
  - Variables to adjust: 7
  - Results Comparison: 7

- Resource Savings** – the time savings is tremendous to achieve the same results.
  - 2000+ iterations would take ~300 hours of a person's time
  - 2000+ iterations with MATLAB/Aspen takes a few hours of computing time – no human time

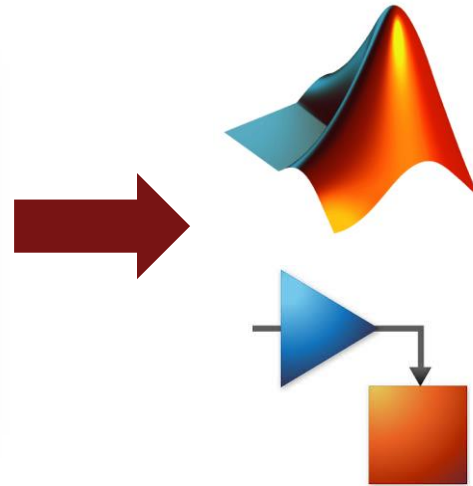
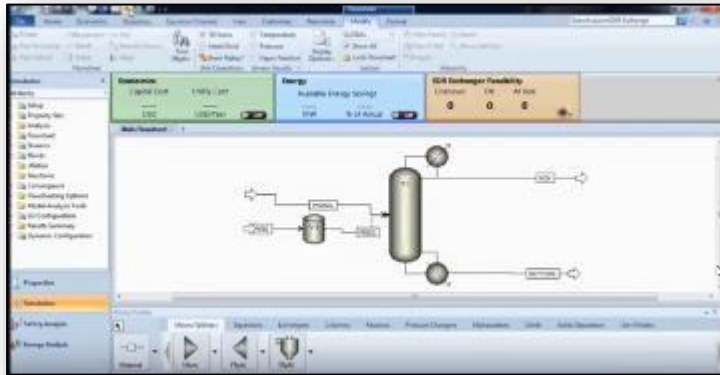
- MATLAB can run the optimization taking weeks to complete
- Case 3:** Dividing Wall
  - Variables to adjust: 1
  - Results Comparison: 1

- Use this approach to optimize existing and new processes
- Achieve capacity gains and lower cost configurations

# Connecting to process simulators

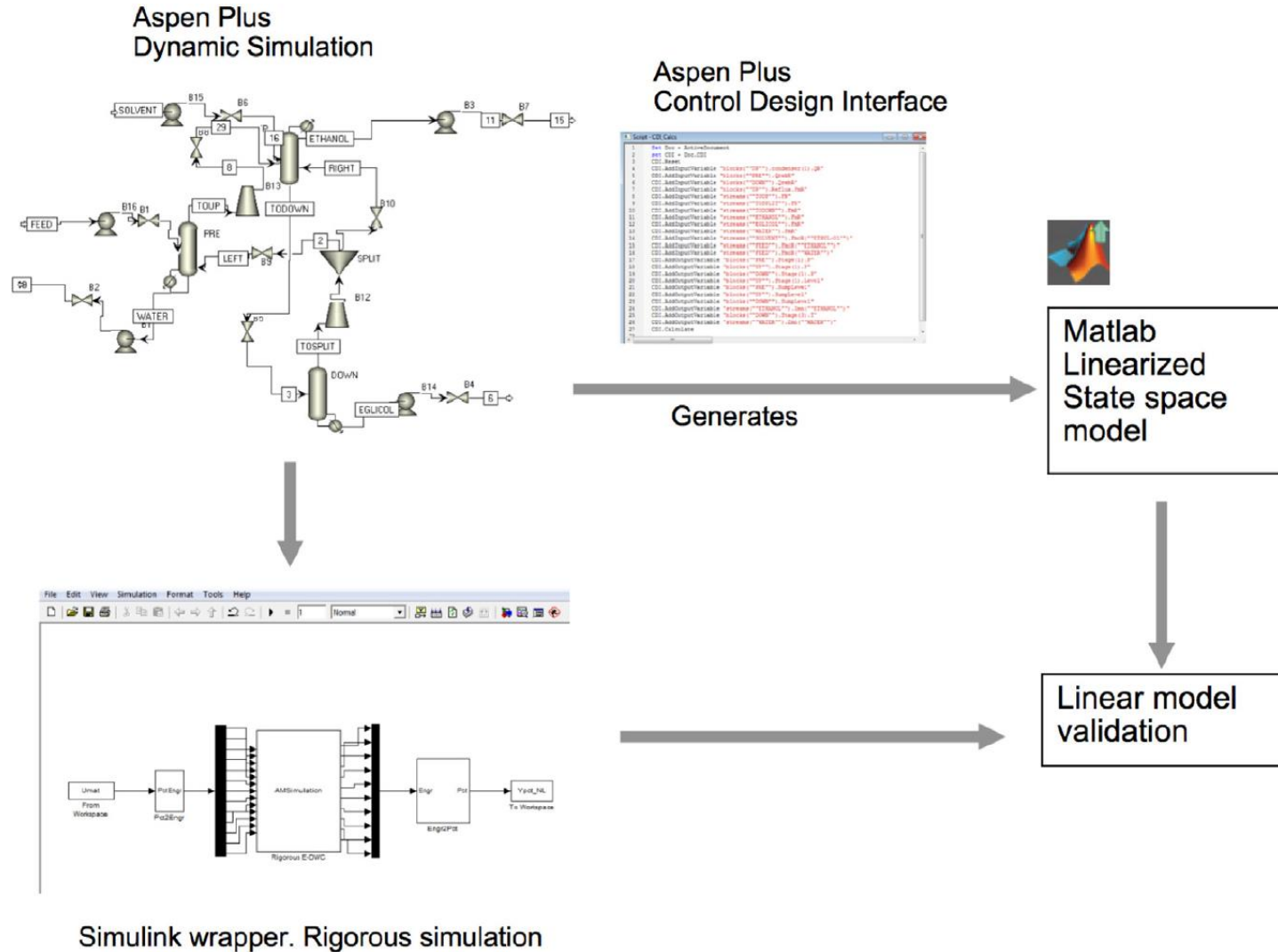
## Calling simulators from MATLAB

- Using native integration





# Import Aspen Plus Dynamics models into Simulink to develop your control strategy



# Import Aspen Plus Dynamics models into Simulink to develop your control strategy

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- « Documentation Home
- « Model Predictive Control Toolbox
- « MPC Design
- « Simulation

**Design and Cosimulate Control of High-Fidelity Distillation Tower with Aspen Plus Dynamics**

ON THIS PAGE

- Distillation Tower
- Build High-Fidelity Plant Model in Aspen Plus Dynamics
- Linearize Plant Using Aspen Plus Control Design Interface
- Create Scaled and Reduced LTI State-Space Model
- Test Accuracy of the Linear Plant Model
- Design Model Predictive Controller
- Cosimulate MPC Controller and Nonlinear Plant
- See Also

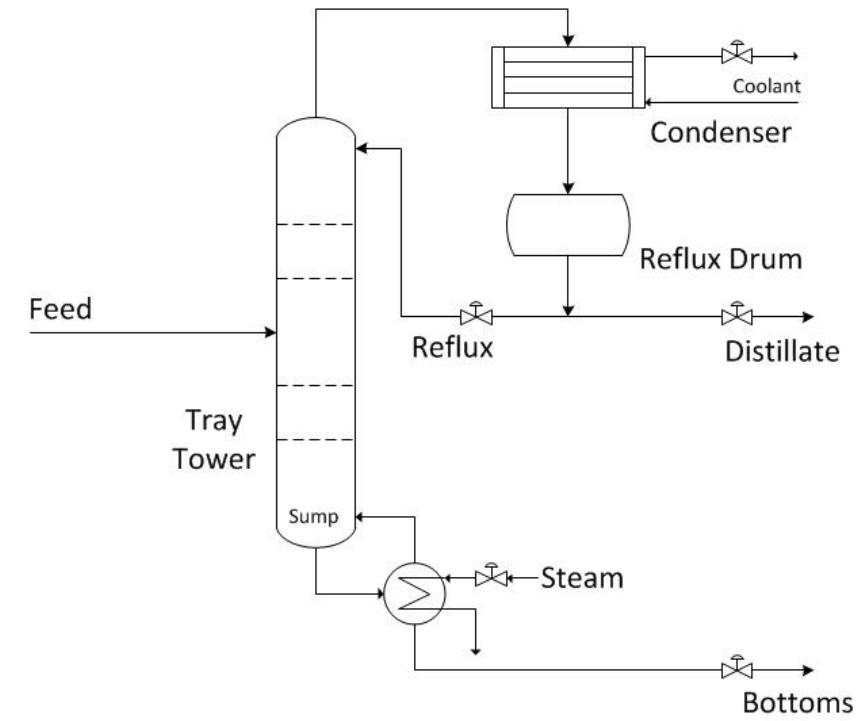
## Design and Cosimulate Control of High-Fidelity Distillation Tower with Aspen Plus Dynamics R2019a

[Try This Example](#)

This example shows how to design a model predictive controller in MATLAB for a high-fidelity distillation tower model built in Aspen Plus Dynamics®. The controller performance is then verified through cosimulation between Simulink and Aspen Plus Dynamics.

### Distillation Tower

The distillation tower uses 29 ideal stages to separate a mixture of benzene, toluene, and xylenes (represented by p-xylene). The distillation process is continuous. The equipment includes a reboiler and a total condenser as shown below:



The distillation tower operates at a nominal steady-state condition:

# Simulink is the preferred platform for APC

## IGCC - Current scenario

### IGCC Power plants in US

- Wabash River Power Station, West Terre Haute, IN
- Polk Power Station, Tampa, FL (350 MW)
- Pinon Rine, Reno, NV (failed)

### Obstacles

- High cost (without carbon regulation)
- Political – Recent emerging IGCC emission controversy
- Supreme court decision requiring Environment Protection Agency to regulate carbon



Wabash



Polk

IGCC Base Case in Aspen Plus

Modify base case

Separate Sub-sections

Prepare for export to Aspen Dynamics

Export Simulation

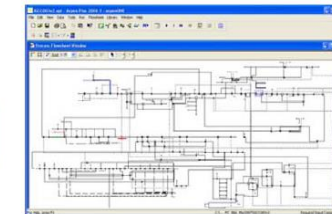
Add simple inventory control PID loops

Identify relevant inputs-outputs

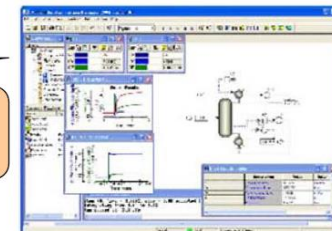
Interface w/ MATLAB/Simulink

Implement control strategies

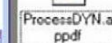
## Plant-wide IGCC Simulation *Aspen Plus to Aspen Dynamics to MATLAB*



Process.bkp



Process.dynf



ProcessDYN.a.pdf



**PLANT-WIDE**

Interconnect sub-sections

Decentralized plant-wide MPC and MMPC

## Using gPROMS with MATLAB

### gO:MATLAB

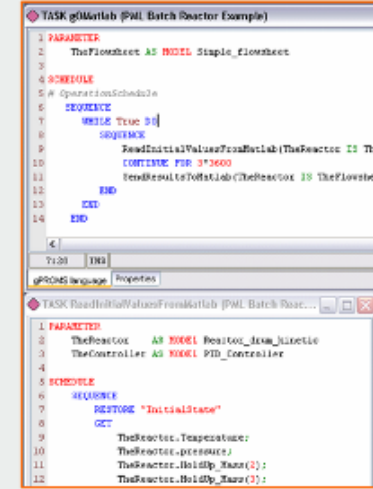
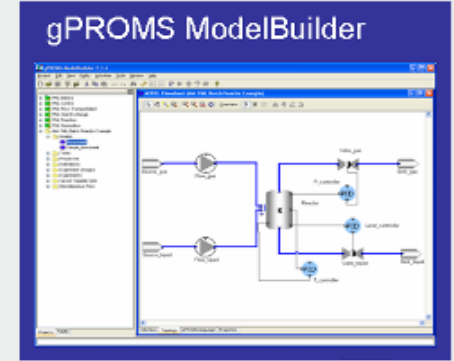
#### The gPROMS Object for MATLAB®

The gPROMS Object for MATLAB® (gO:MATLAB) is a unique and powerful tool that enables control engineers to deploy complex, non-linear gPROMS advanced process models within the widely-used Mathworks MATLAB® environment.

gO:MATLAB allows an entire gPROMS model to be called as a single function from inside MATLAB, enabling you to solve a complex set of algebraic and ordinary and partial differential equations within a single call.

It is of particular benefit where an existing gPROMS process model can be redeployed, thus saving development costs.

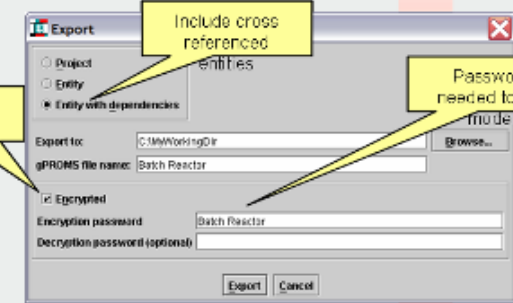
**Step 1:** Develop and test the gPROMS model inside the gPROMS ModelBuilder environment.



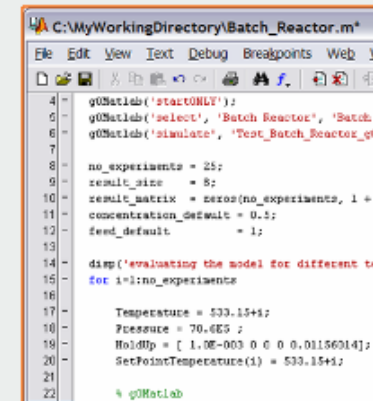
**Step 2:** Create a gPROMS schedule that periodically exchanges relevant data between gPROMS and MATLAB.

**Step 3:** Export the model gPROMS model

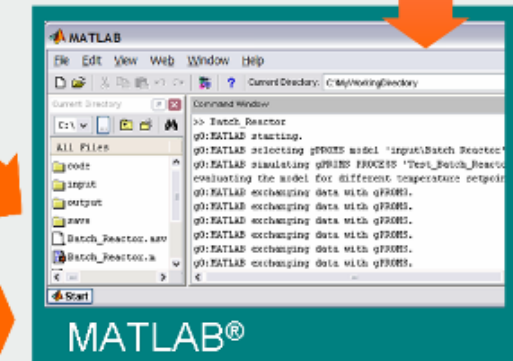
Exported file to be encrypted



**Step 4:** Create a MATLAB script file (e.g. cstr.m)



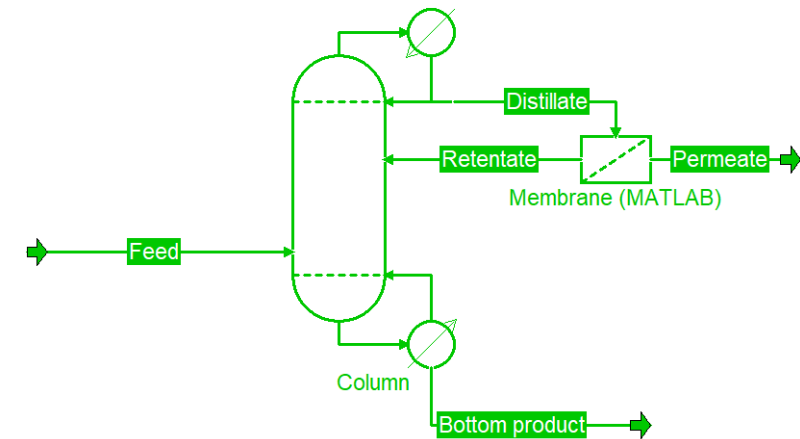
**Step 5:** Execute the gPROMS model from within MATLAB.



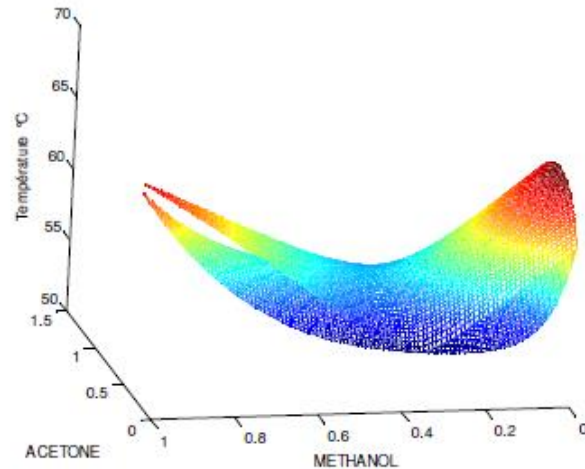
# Connecting to process simulators

## Embedding MATLAB in simulators

- Using CAPE-OPEN



# CAPE-OPEN interfaces allow engineers to leverage the strengths of each platform

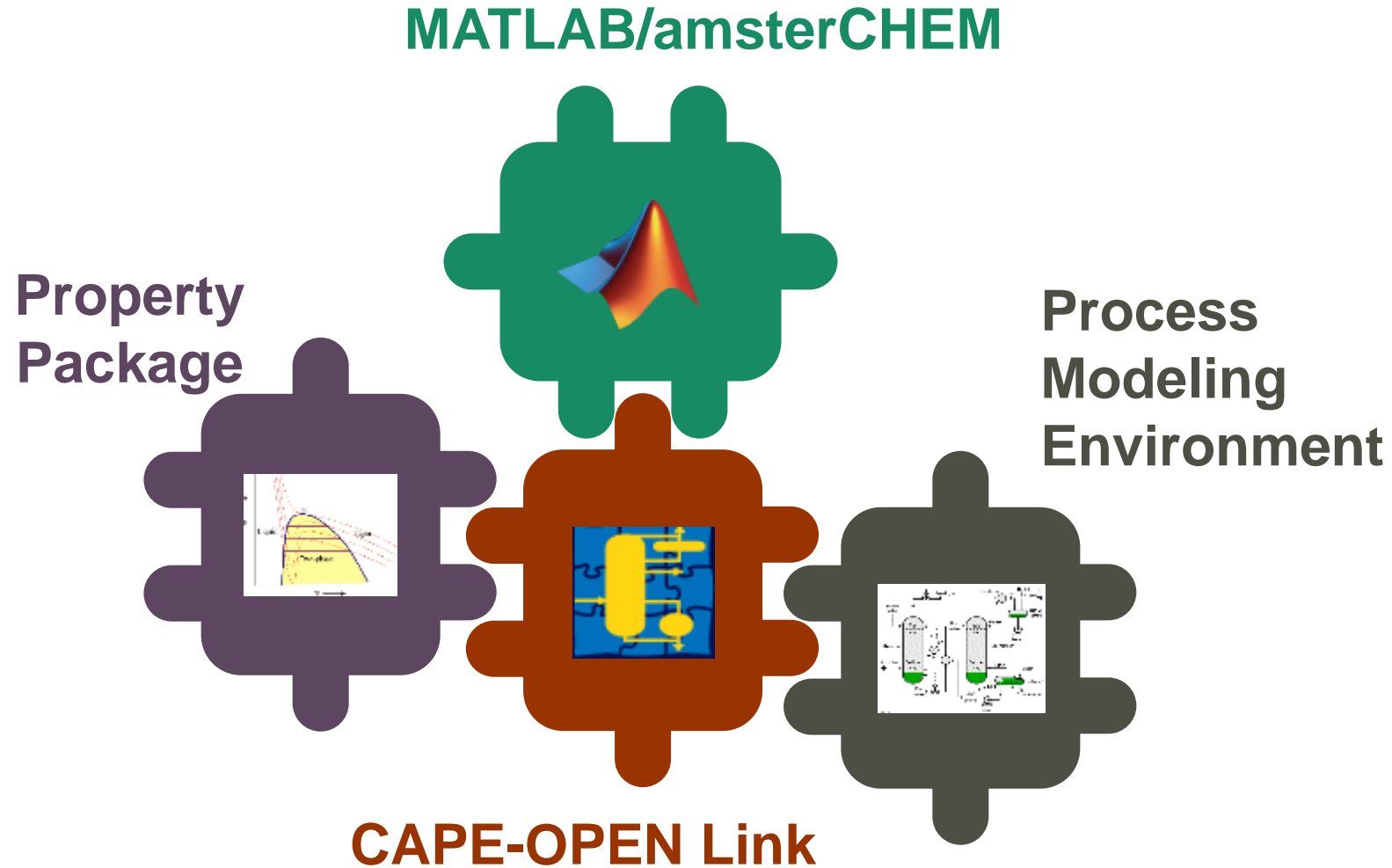


Visualizing a two-phase, three component mixture in MATLAB via Simulis®

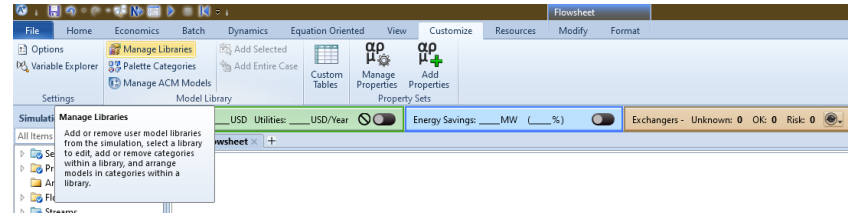
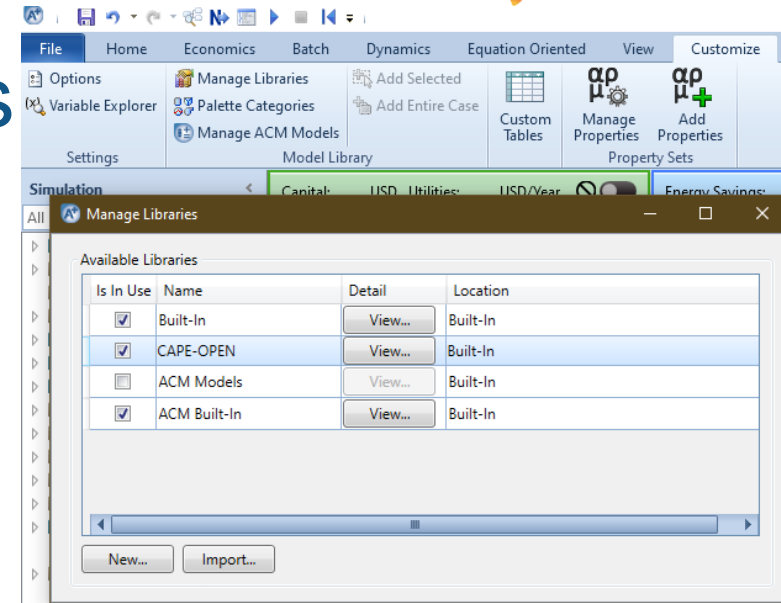
- AspenTech(Aspen Plus, HYSYS)
- ANSYS
- Schneider Electric (PRO/II, ROMeO)
- KBC (Petro-Sim)
- PSE (gPROMS)
- HTRI (Xchanger suite)
- Many more....

**Some of the many organizations that support CAPE-OPEN interfaces**

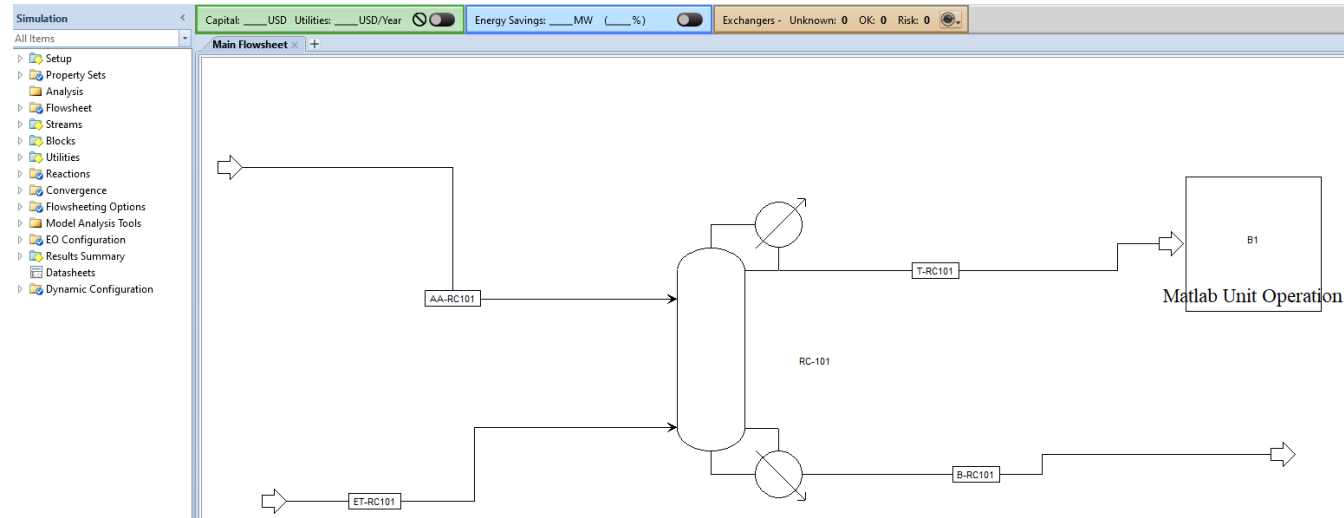
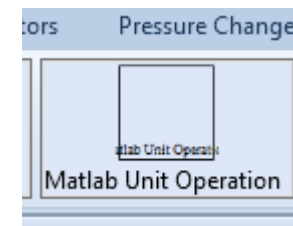
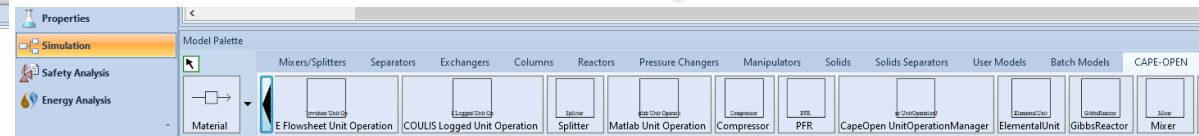
# MATLAB supports CAPE-OPEN interface through a third-party package



# Embedding MATLAB models in Aspen Plus



MatlabCapeOpenUnitOperation.2.0.0.7.exe



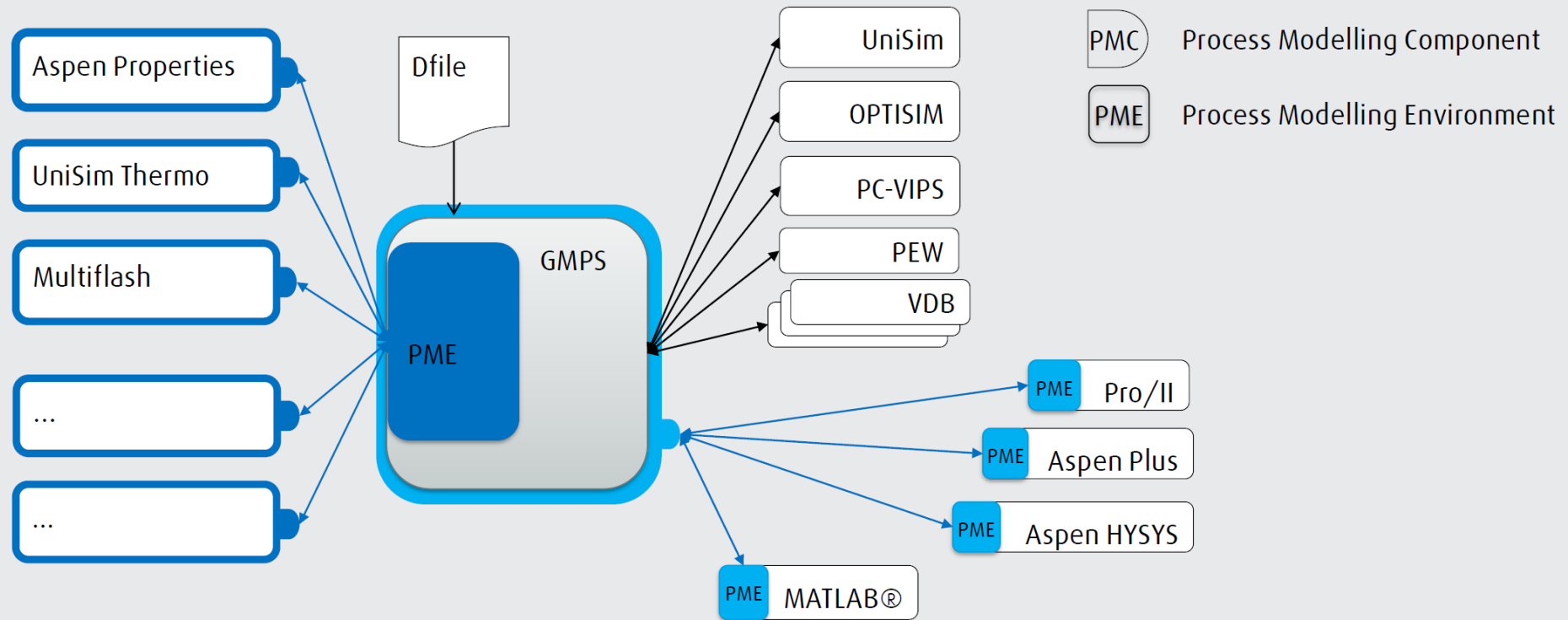


# Linde uses MATLAB unit operations with CAPE-OPEN

## CAPE-OPEN Thermo Interfaces to Linde's Thermo Package



Lehrstuhl für  
Anlagen- und Prozesstechnik

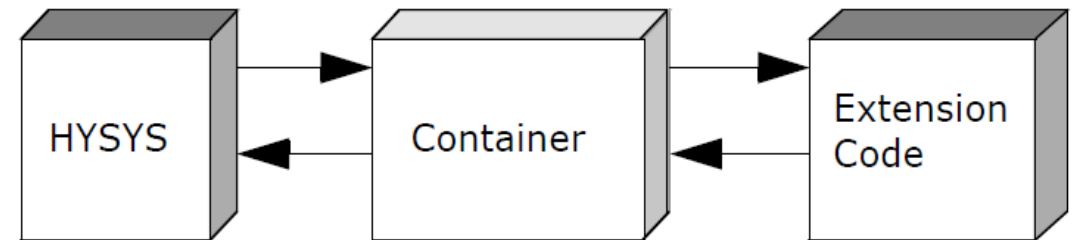


- [Usage at Linde](#)
- [University of Utah](#) use MATLAB with CAPE-OPEN for a catalytic membrane reactor model
- [Norwegian University of Science and Technology \(NTNU\)](#) use MATLAB models wrapped as [CAPE-OPEN Unit](#) Operations
- [Usage at](#) Technical University of Madrid

# Connecting to process simulators

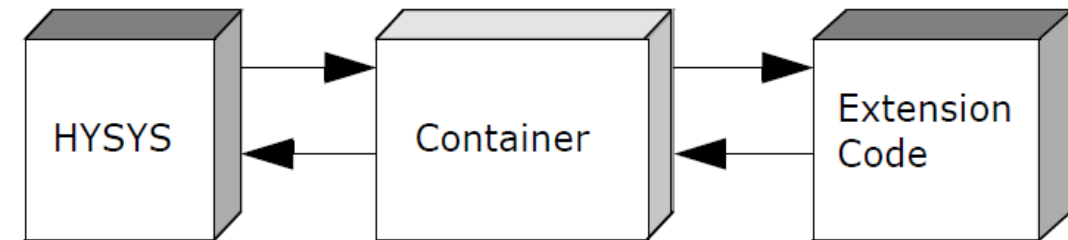
## Embedding MATLAB in simulators

- Using HYSYS extension container



# Using the HYSYS extension structure

- Create a dll from MATLAB code using MATLAB Coder
- Create an Extension Definition File (EDF) using the HYSYS Extension View Editor supplied with HYSYS
- Register dll with EDF
- More details in sections 3.5, 3.6 and chapter 4 of the [HYSYS customization guide](#)



# Which method do you plan to use?

## Calling simulators from MATLAB

- Using ActiveX automation server
- Using native integration

## Embedding MATLAB in simulators

- Using CAPE-OPEN
- Using HYSYS extension container

