Adding automation and data analysis to process simulators with MATLAB

Samvith Rao

Samvith Rao

- B.S, M.S in Chemical Engineering
  - IIT Madras
  - Honeywell

- Reliance Industries Limited, India
  - Process Technologist
  - Field Engineer

- MBA
  - UNC Chapel Hill

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MathWorks

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Privately held
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MathWorks

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.

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

MathWorks® 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.

Gartner peerinsights customers' choice 2020 ™

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

Disclaimer: Gartner, Gartner Peer Insights 'Voice of the Customer': Data Science and Machine Learning Platforms, July 2020. This graphic was published by Gartner, Inc. as part of a larger research document and should be evaluated in the context of the entire document. The Gartner document is available upon request from MathWorks.

IEEE Top Programming Languages 2020

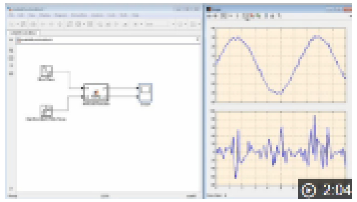
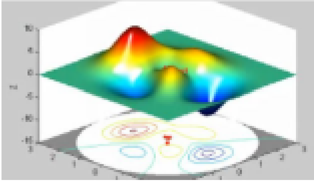
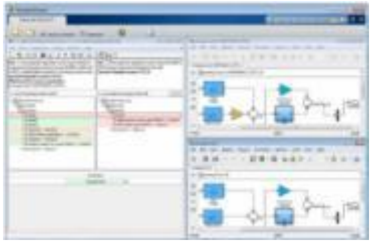
Rank	Language	Type	Score
1	Python		100.0
2	Java		95.3
3	C		94.6
4	C++		87.0
5	JavaScript		79.5
6	R		78.6
7	Arduino		73.2
8	Go		73.1
9	Swift		70.5
10	Matlab		68.4

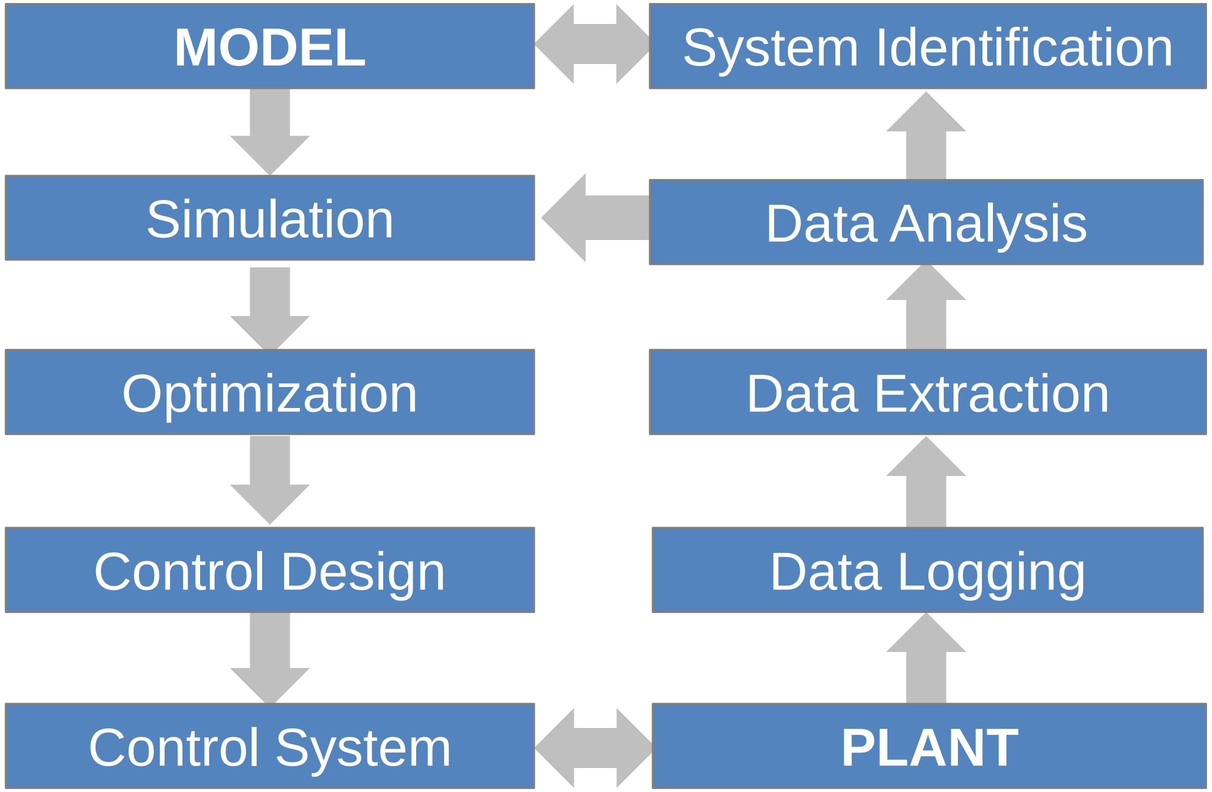
https://spectrum.ieee.org/at-work/tech-careers/top-programming-language-2020

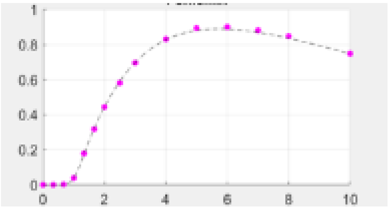
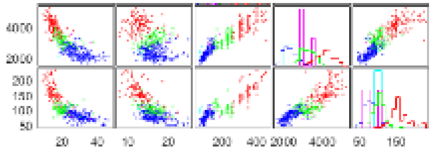
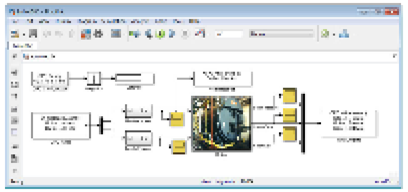
Process Engineering Workflow

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

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

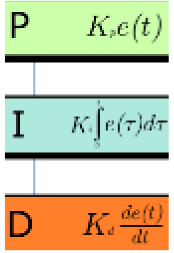




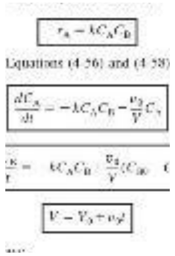




MathWorks provides a comprehensive suite of software tools to support this workflow.

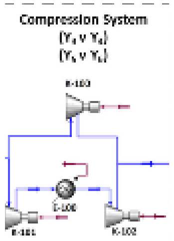
Use cases for integrating MATLAB with process simulators



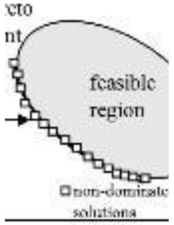
Control Strategy



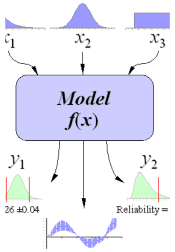
Custom Unit Operations



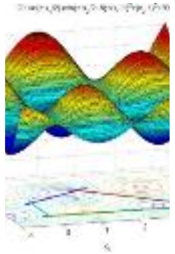
Scenario modeling



Multi-objective optimization

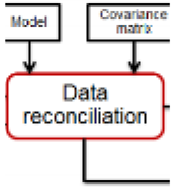


Sensitivity analysis

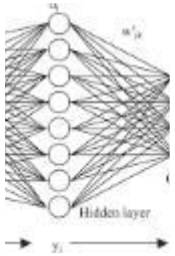


Dynamic optimization

Automating repetitive tasks



Pre-processing data



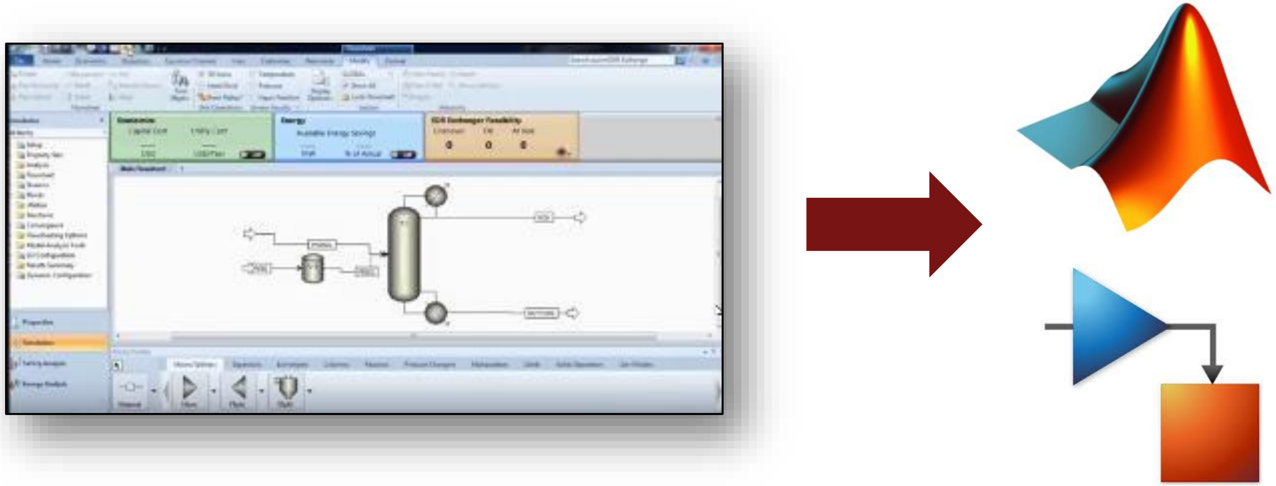
Machine Learning

Some examples

Connecting to process simulators

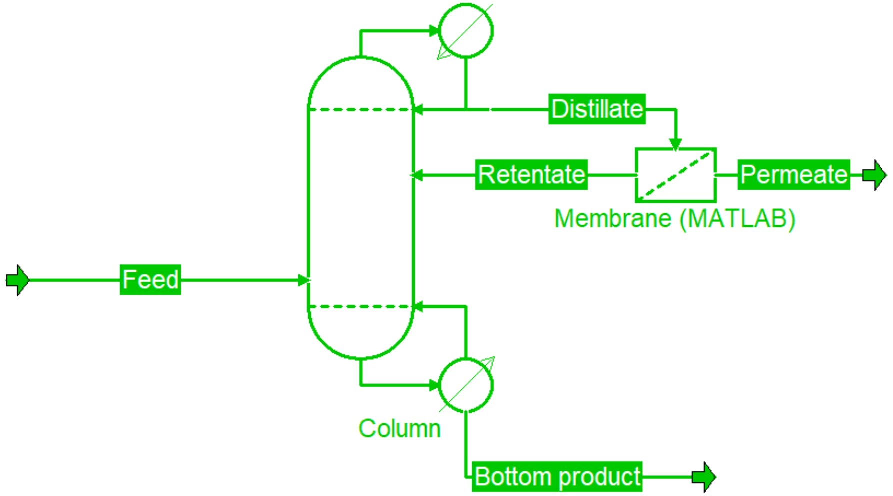
Calling simulators from MATLAB

- Using ActiveX automation server
- Using native integration



Embedding MATLAB in simulators

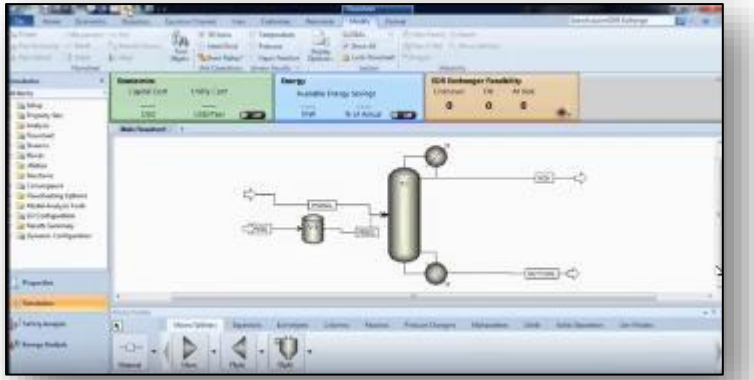
- Using CAPE-OPEN
- Using HYSYS extension container



Connecting to process simulators

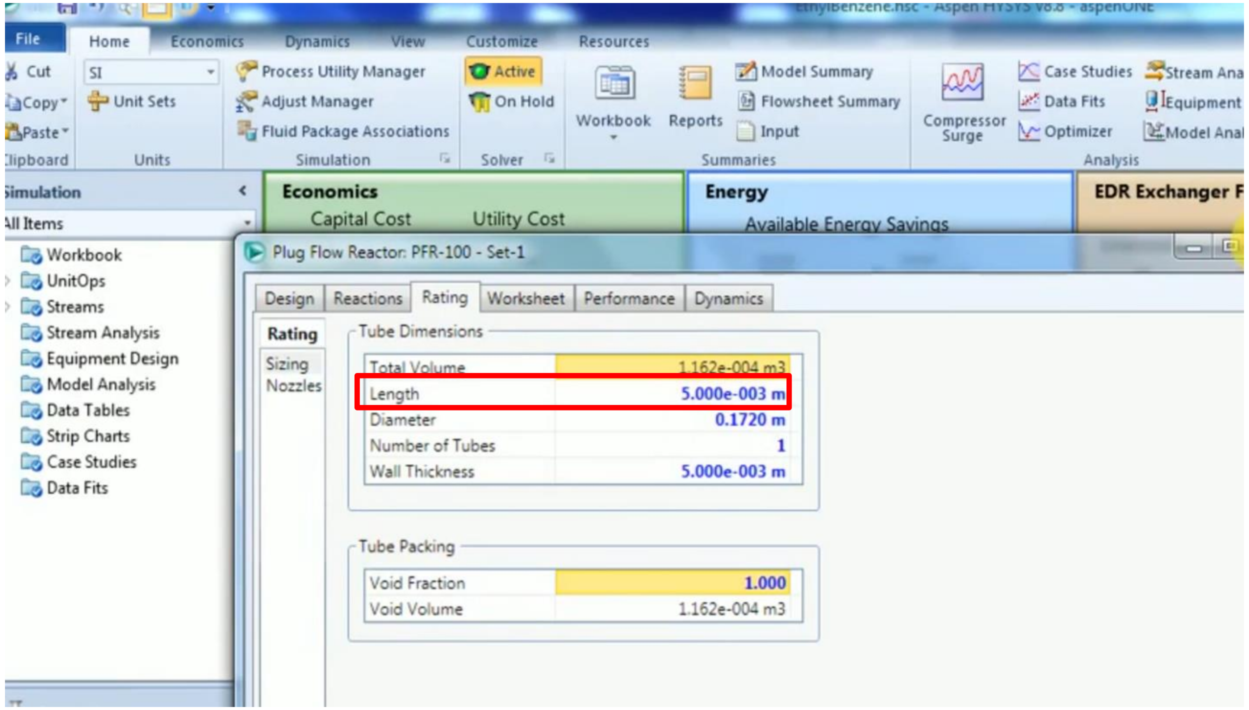
Calling simulators from MATLAB

- 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;
```



[Link to Download]

Connecting MATLAB to Aspen Plus

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File Exchange

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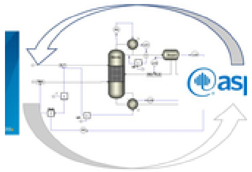


Aspen Plus - Matlab Link

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

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

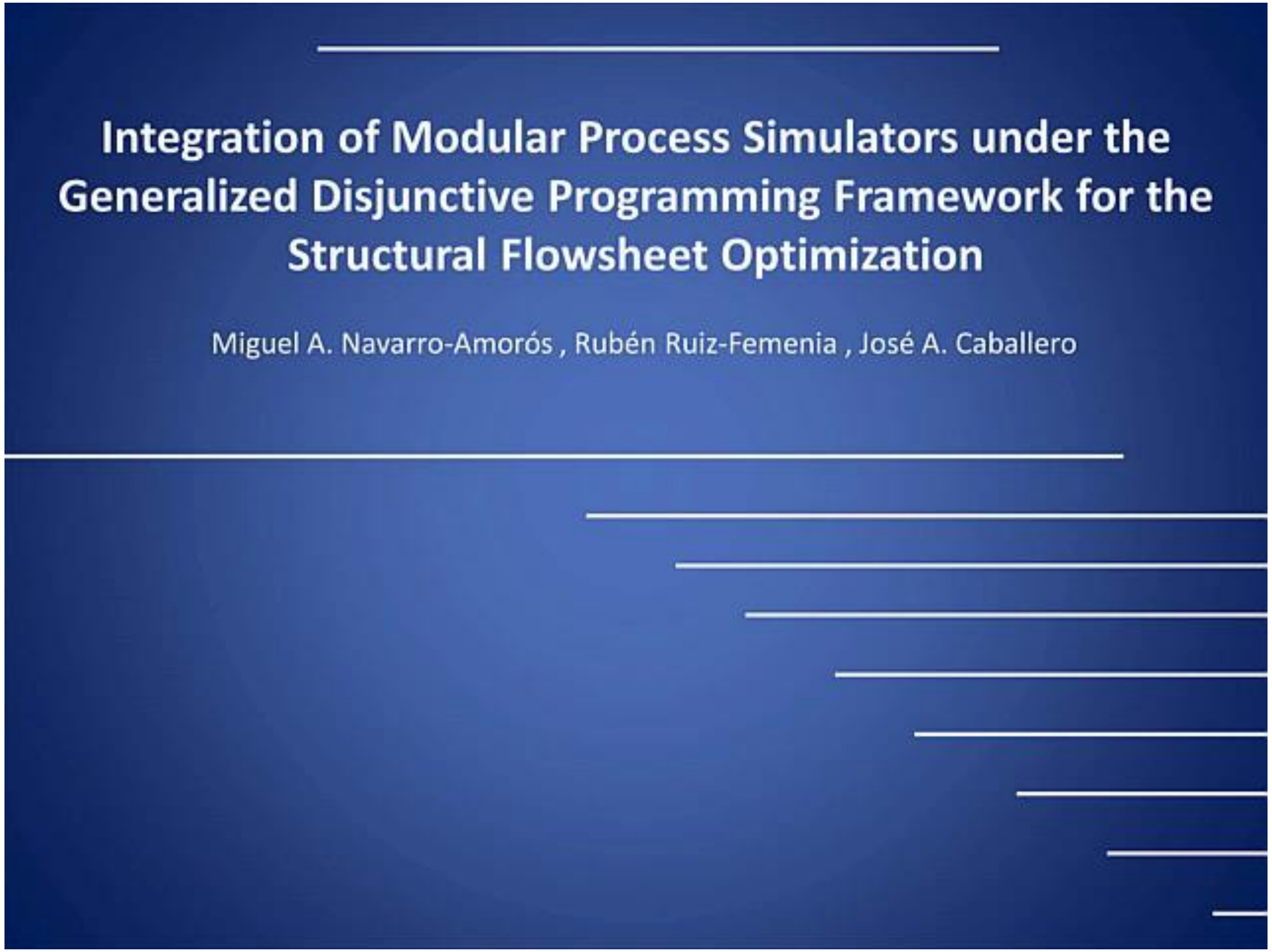
Simulation file (Aspen Plus V.10.0) in: https://drive.google.com/open?id=1oSqqMj11h3NJIHPlhzCeok9baaH4PHnC

Requires Aspen Plus V.10.0 software

Google ‘Aspen Plus MATLAB’

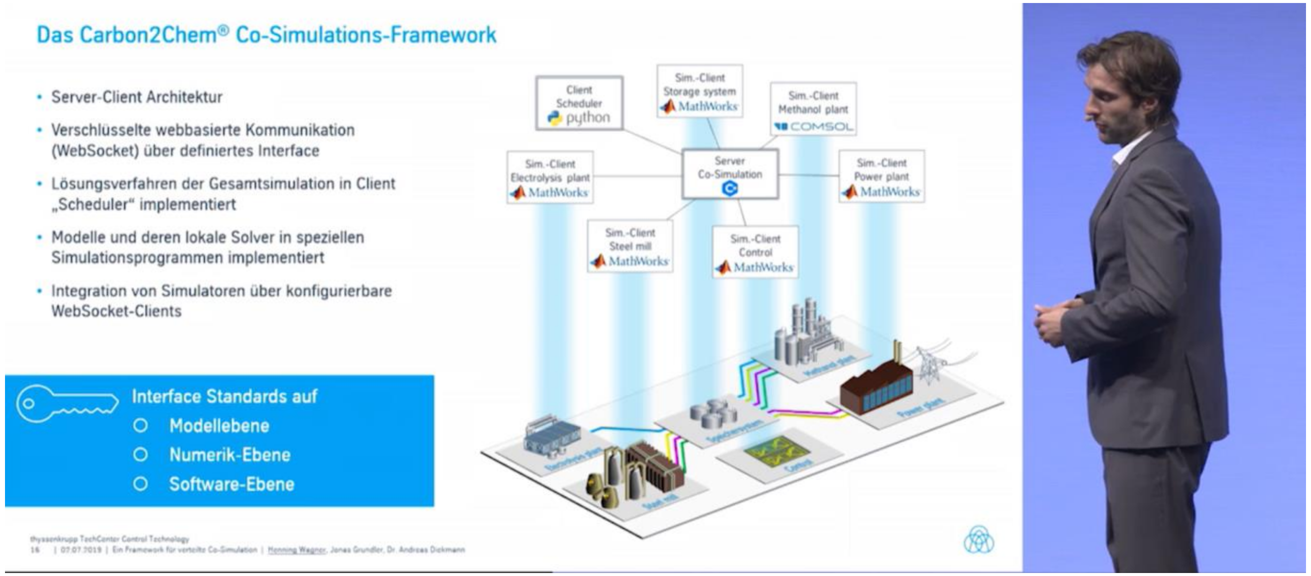
Link to Download

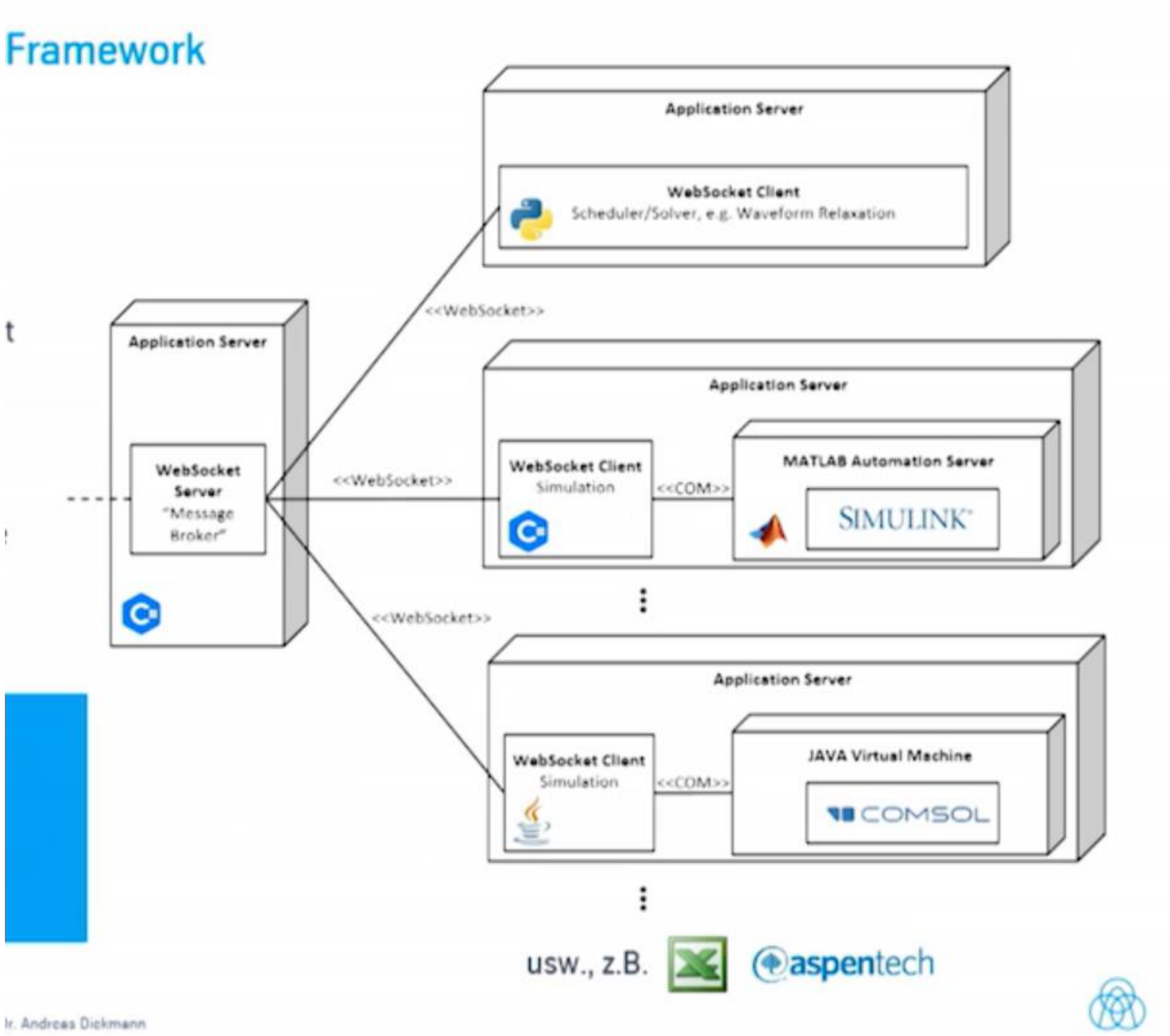
Flowsheet structure optimization with MATLAB and HYSYS



Link to paper

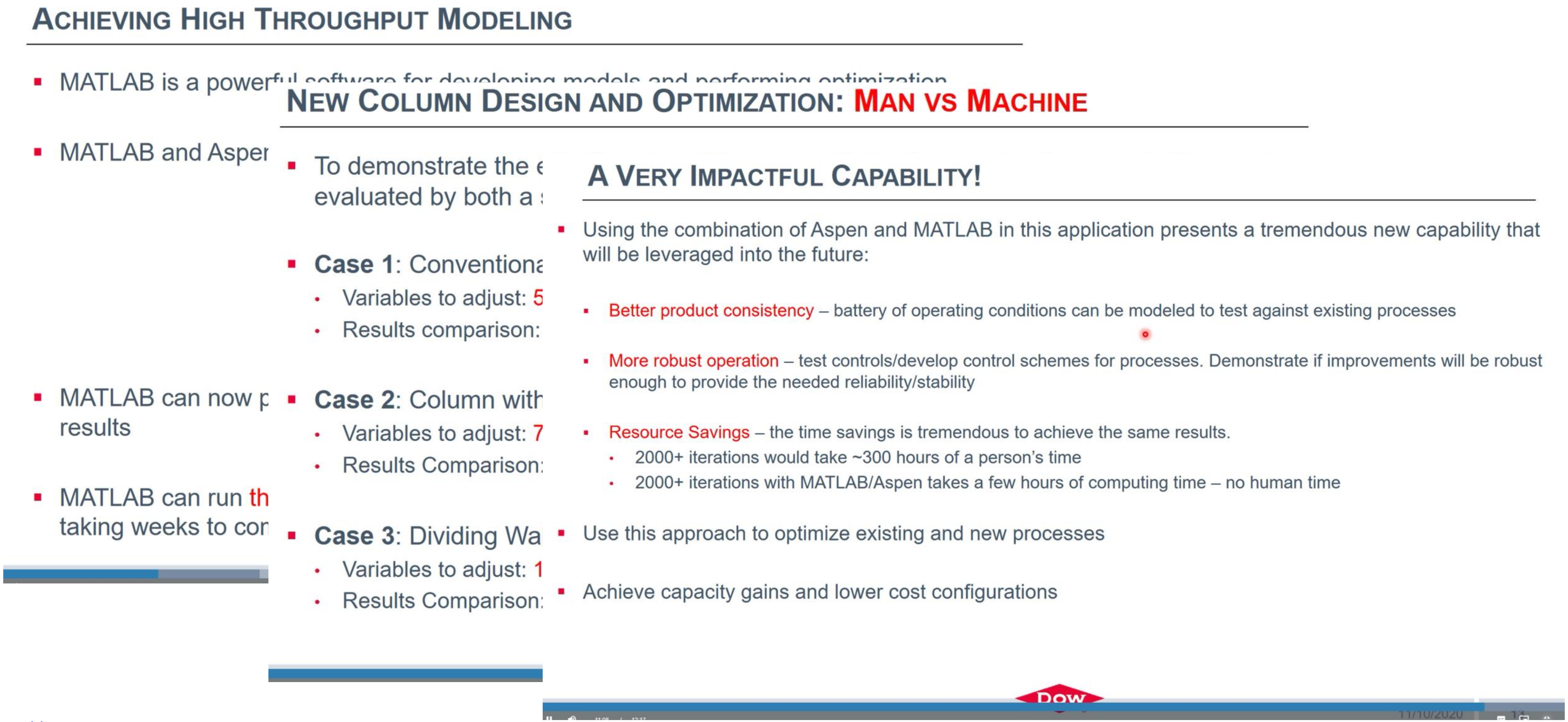
Thyssenkrupp co-simulates MATLAB with Aspen Plus and COMSOL to model CCU plant





[Link to user story]

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

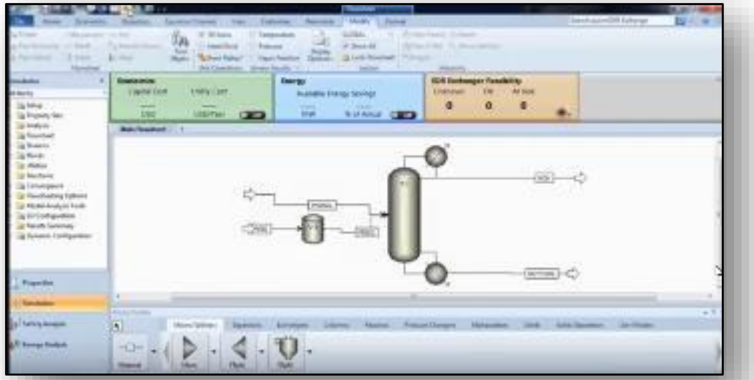


Link to video

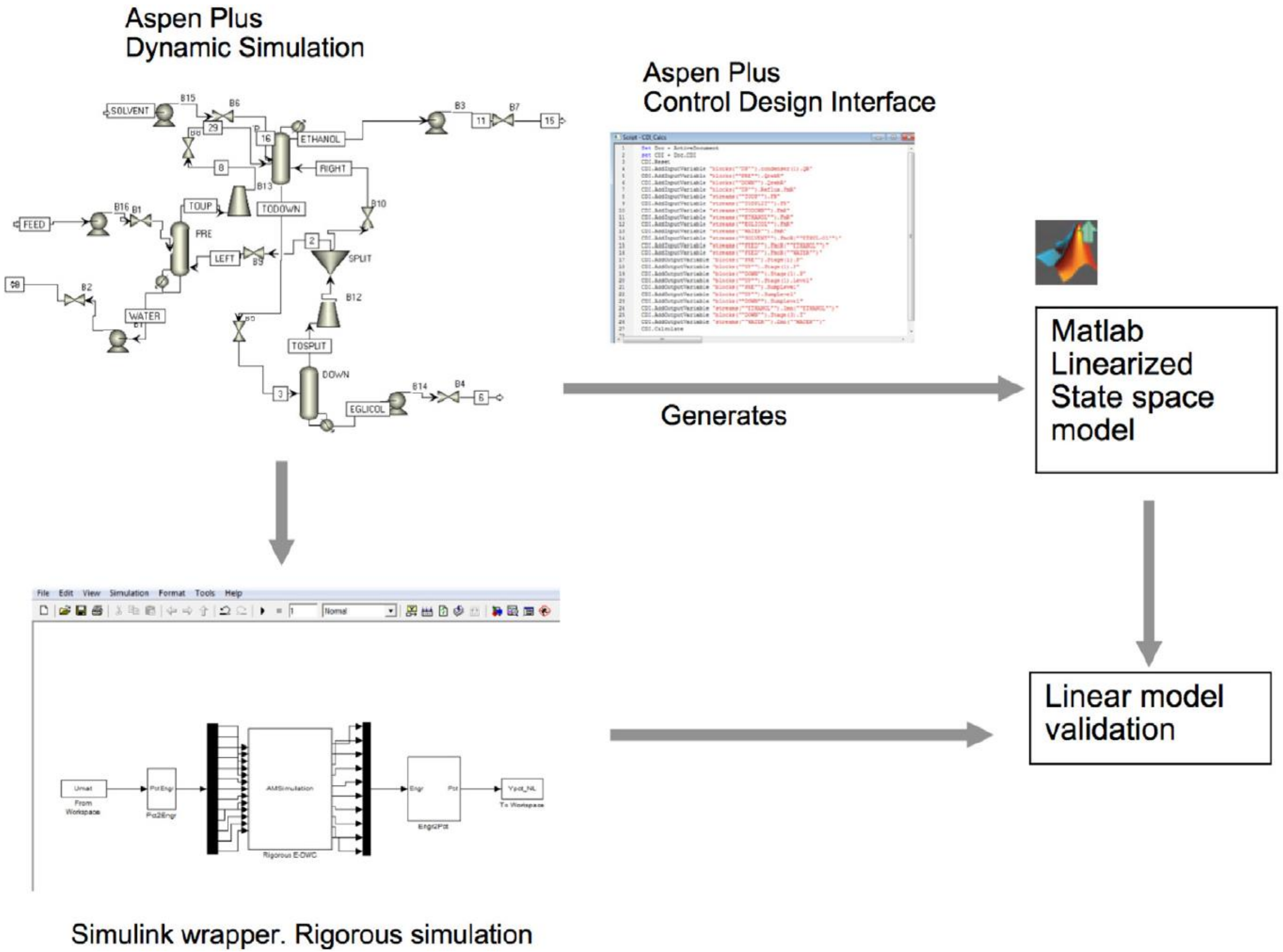
Connecting to process simulators

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

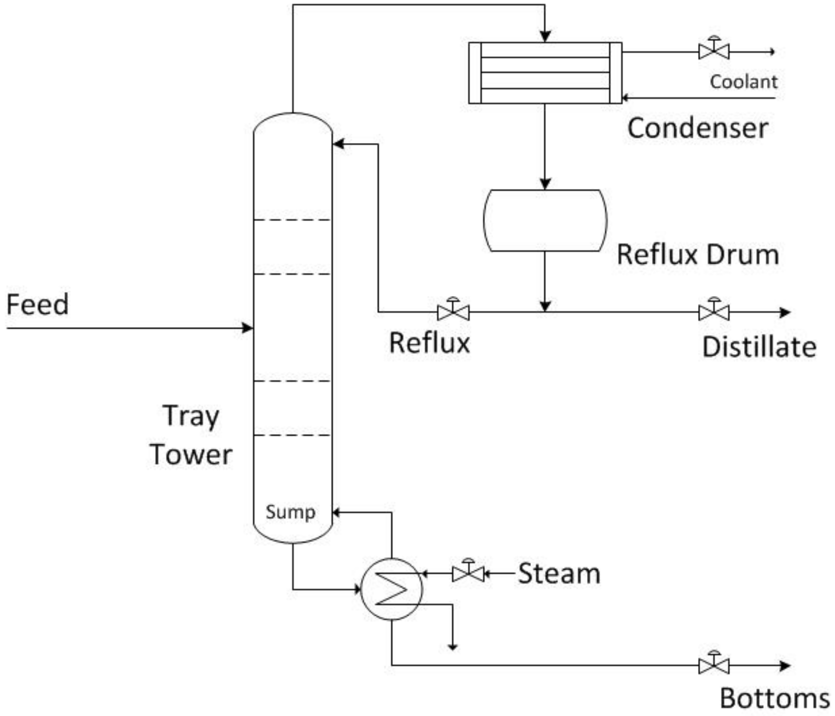
R2019a

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.

Try This Example

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:

[Link to documentation](#)

Simulink is the preferred platform for APC

IGCC - Current scenario

IGCC Power plants in US

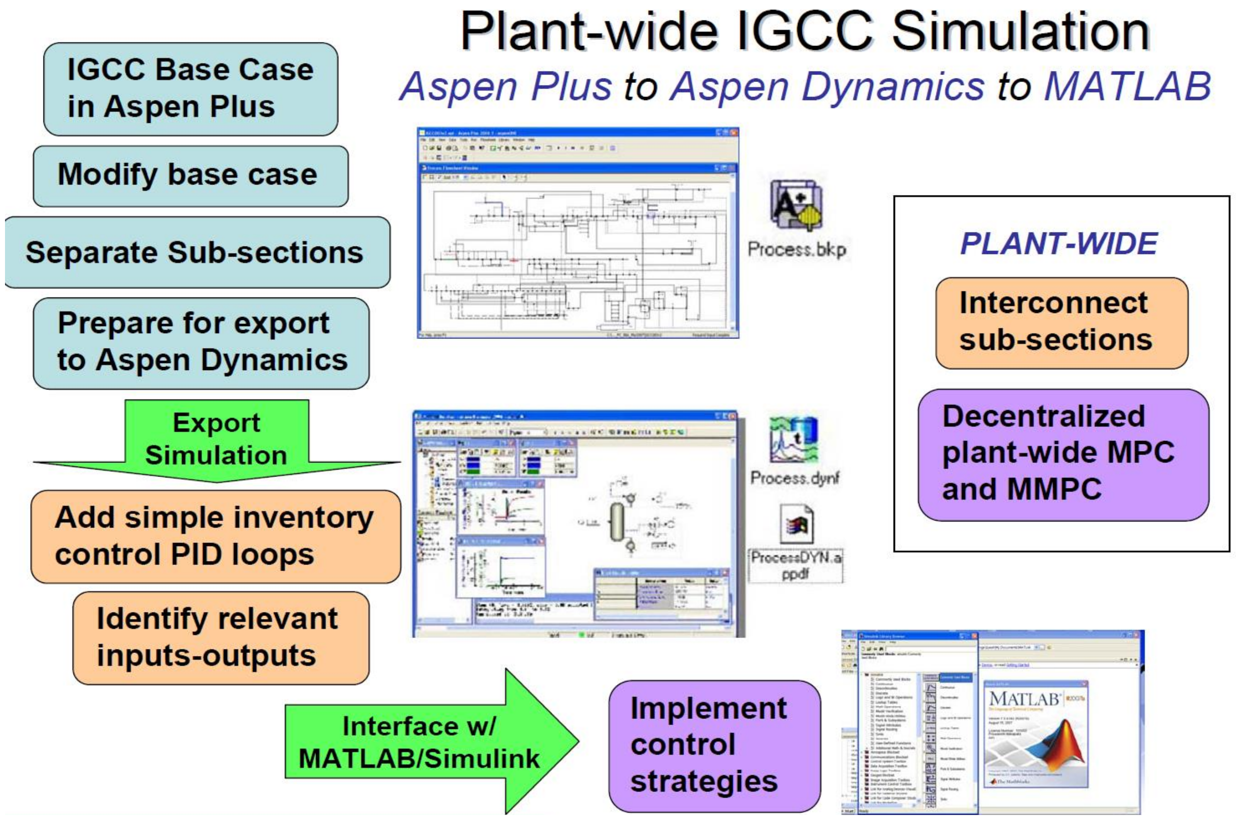
- Wabash River Power Station, West Terre Haute, IN
- Polk Power Station, Tampa, FL (350 MW)
- Pinon Rine, Reno, NV (failed)

Obstacles

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

Wabash

Polk



Using gPROMS with MATLAB

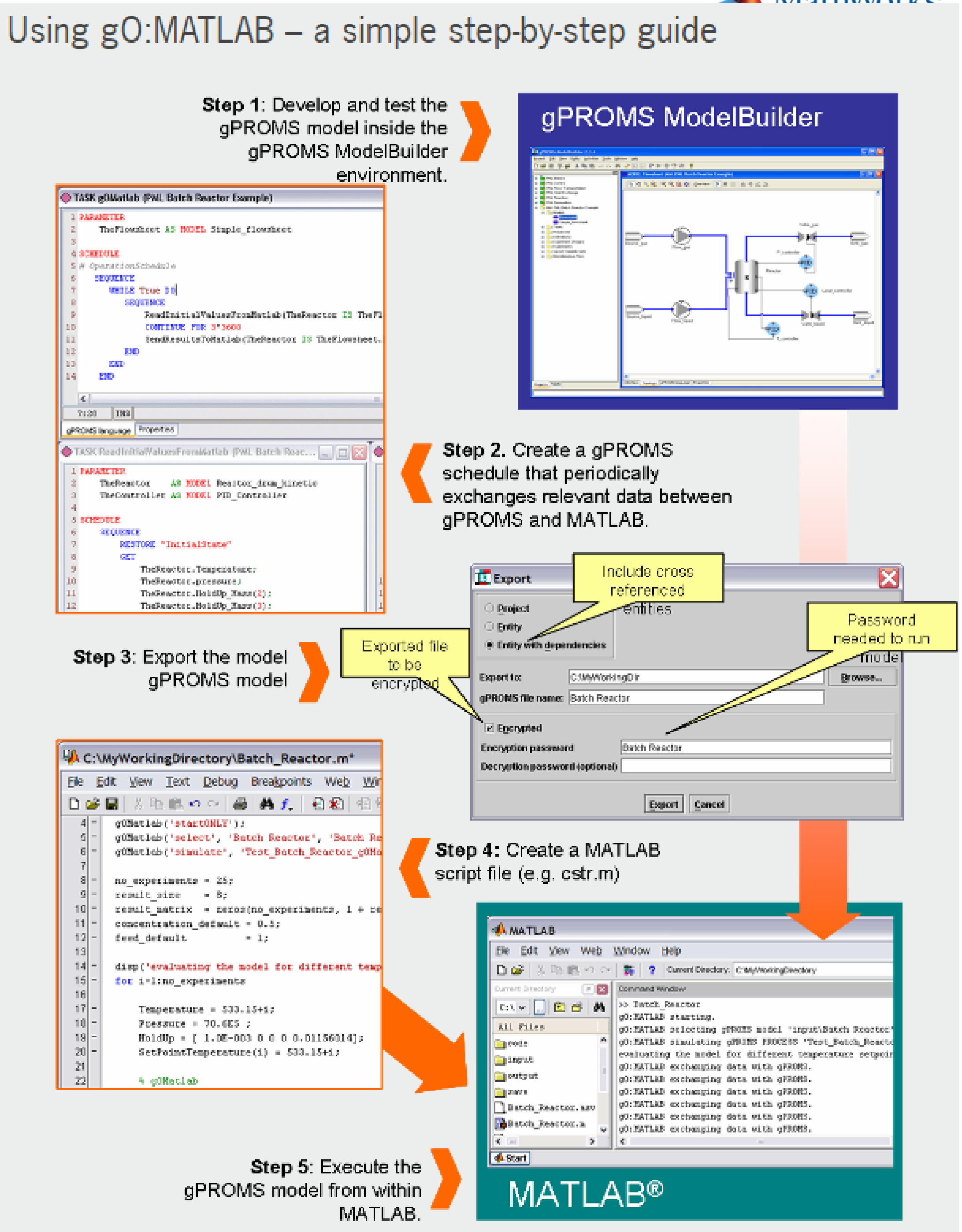
gO:MATLAB

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.

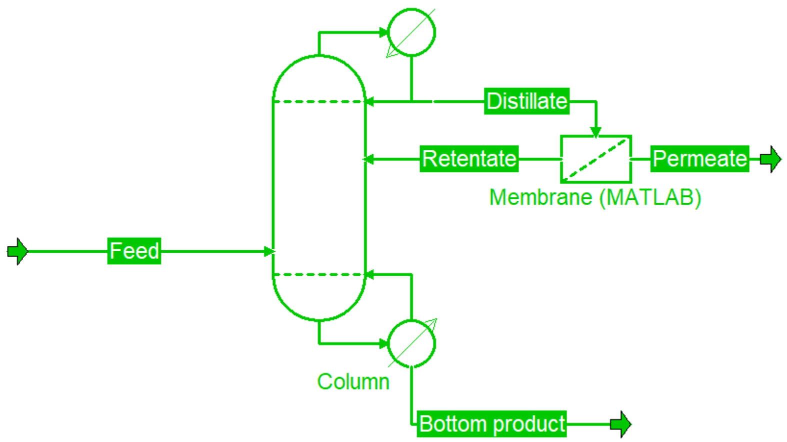


[Link to download]

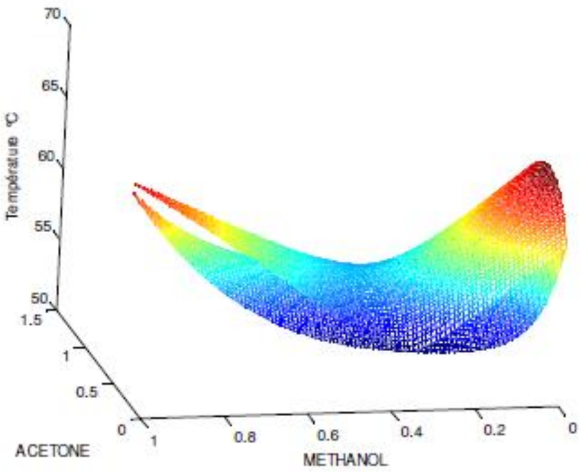
Connecting to process simulators

Embedding MATLAB in simulators

– Using CAPE-OPEN



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



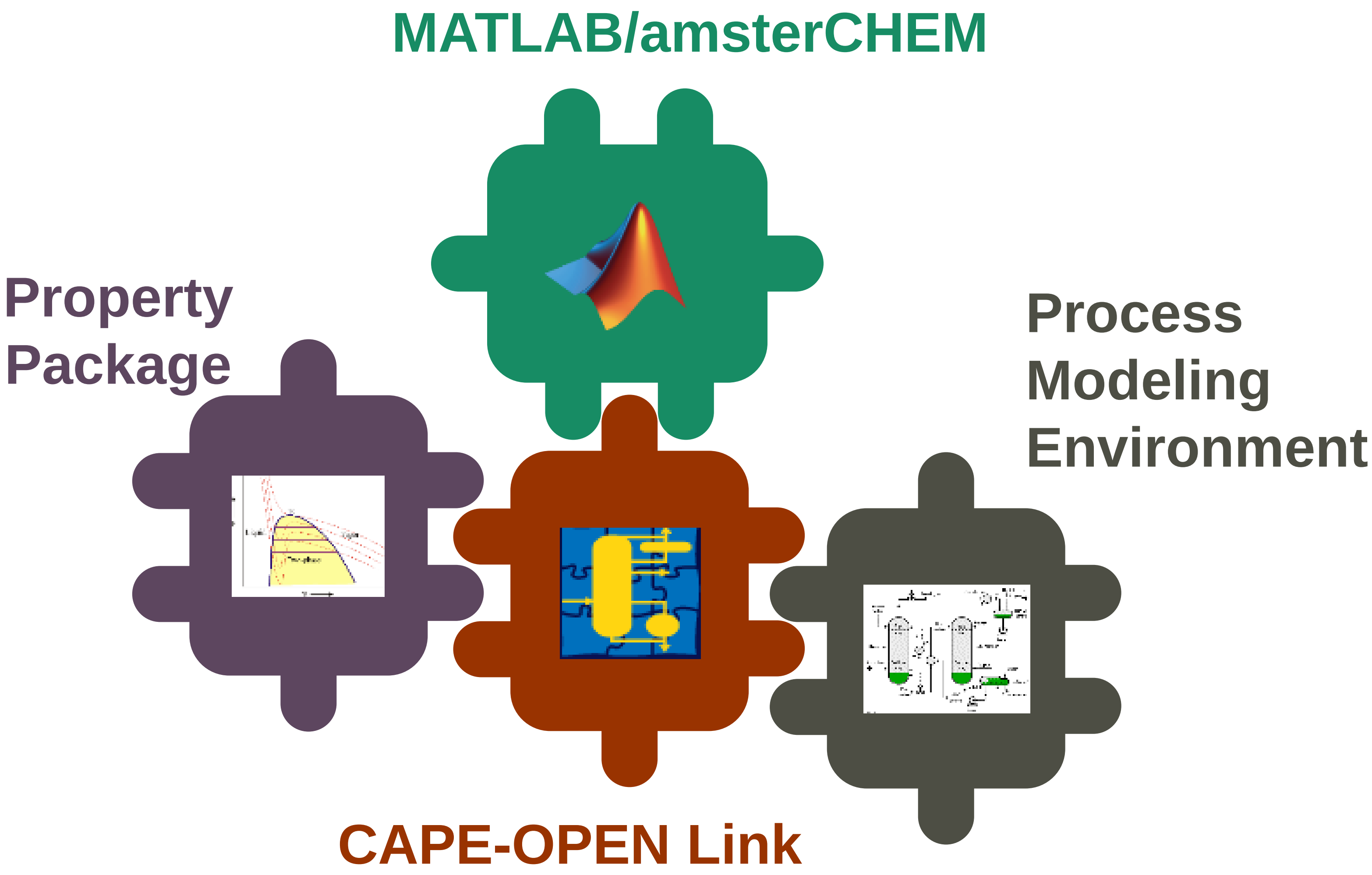
Visualizing a two-phase, three component mixture in MATLAB via Simulis®

- 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

http://www.colan.org/

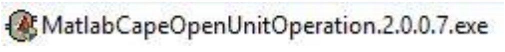
MATLAB supports CAPE-OPEN interface through a third-party package

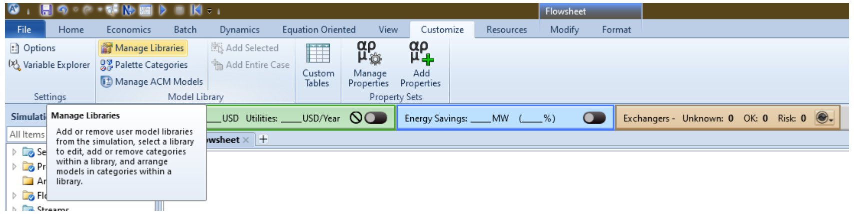


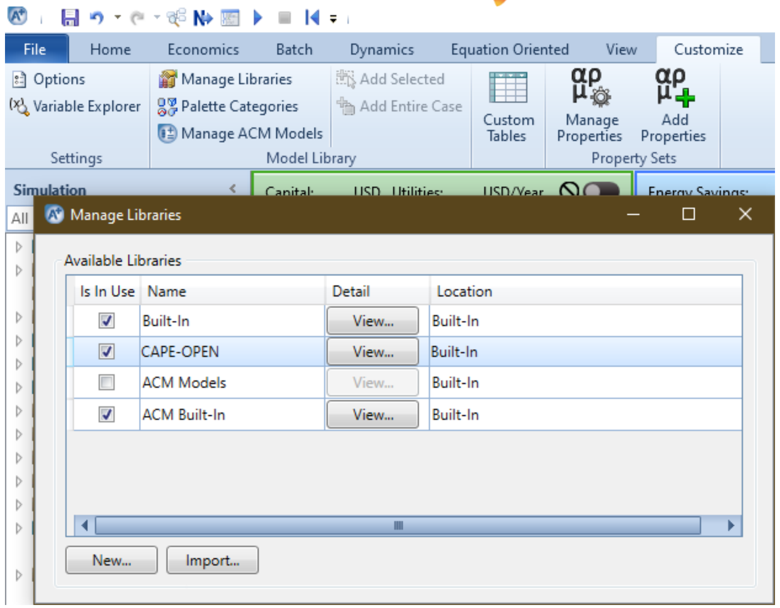
https://www.amsterchem.com/matlabunitop.html

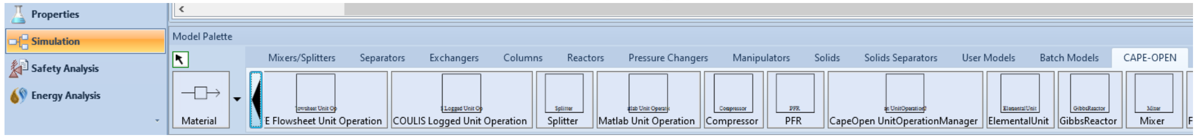
MathWorks®

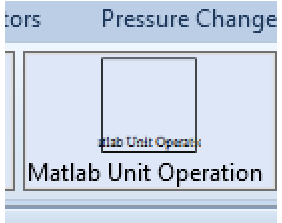
Embedding MATLAB models in Aspen Plus

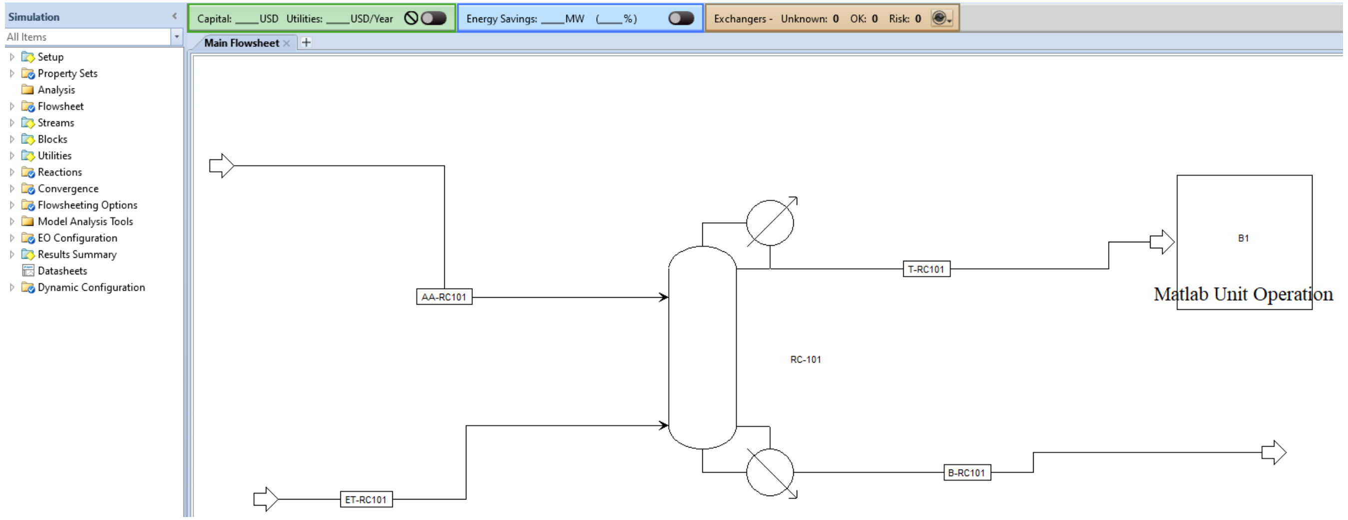






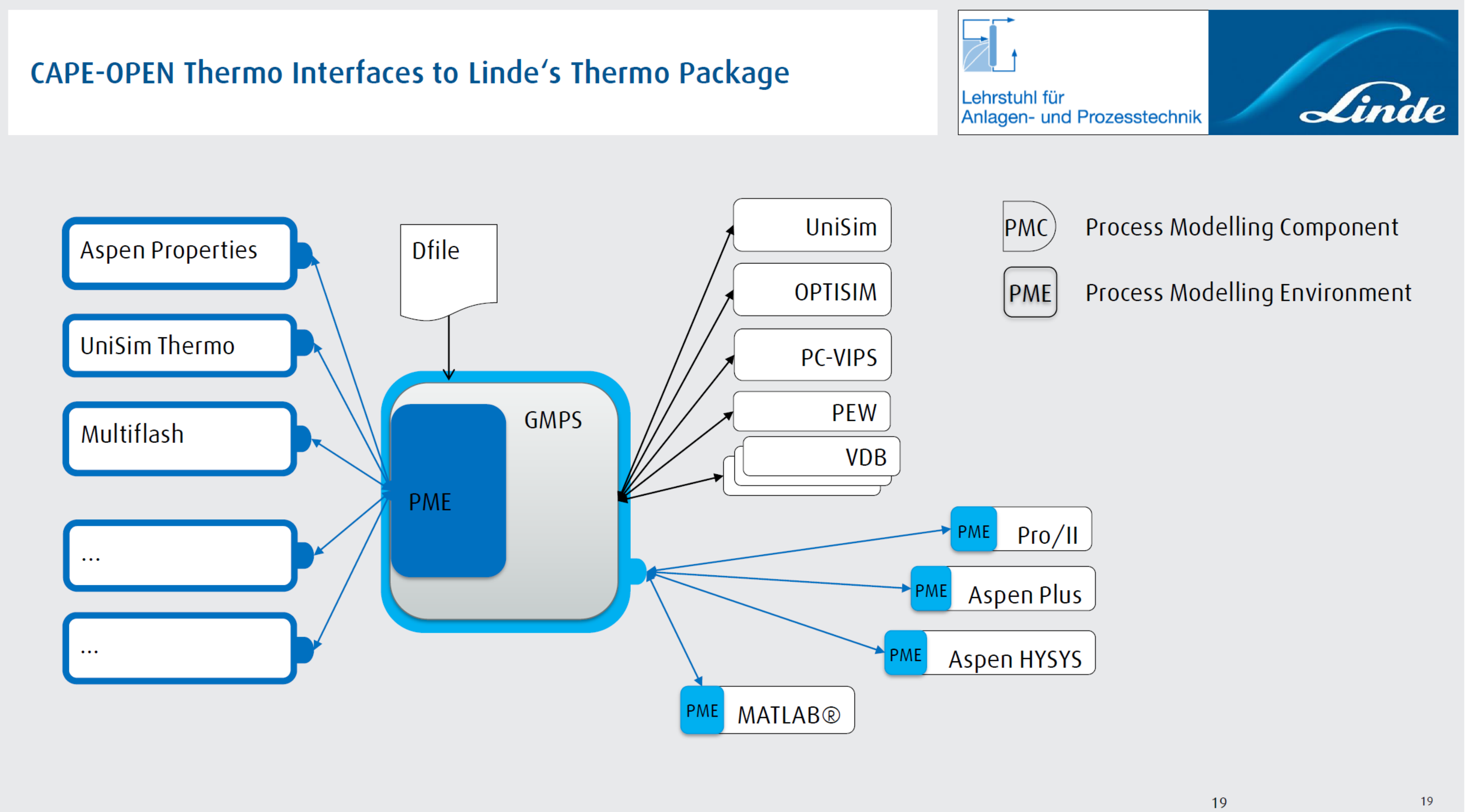






Link to Download

Linde uses MATLAB unit operations with CAPE-OPEN

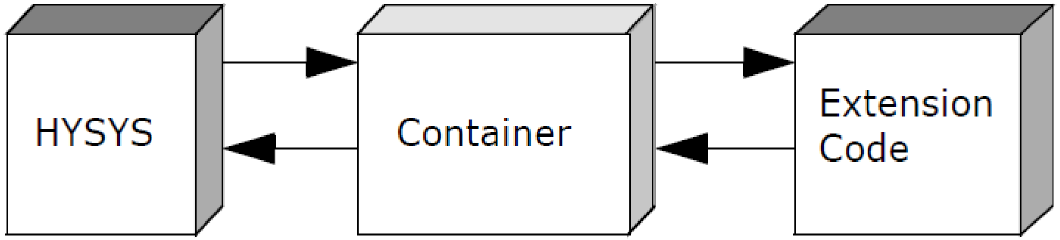


- Usage at Linde
- University of Utah use MATLAB with CAPE-OPEN for a catalytic membrane reactor model
- Norwegian University of Science and Technology (NTNU) use MATLAB models wrapped as CAPE-OPEN Unit Operations
- Usage at Technical University of Madrid

Connecting to process simulators

Embedding MATLAB in simulators

- Using HYSYS extension container



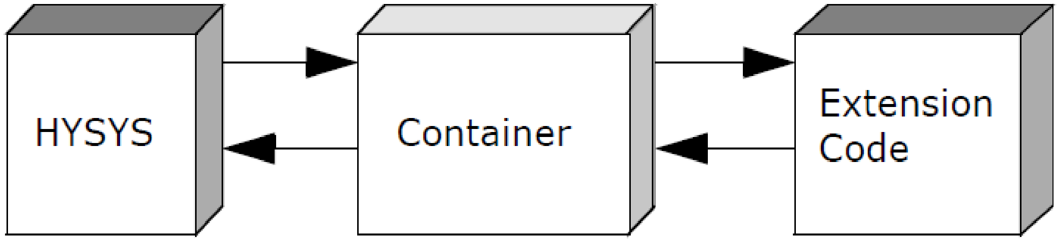
Using the HYSYS extension structure

- 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

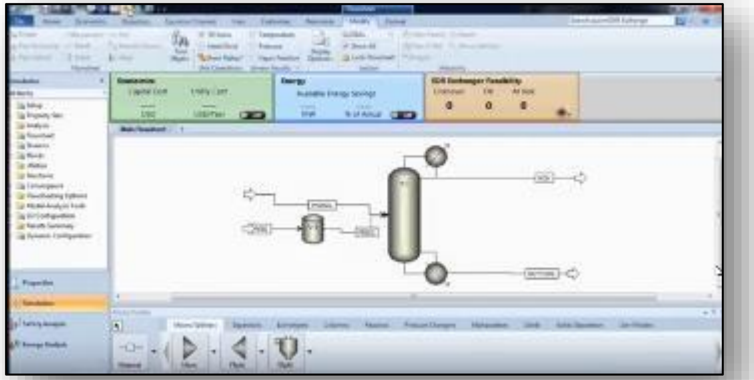
- More details in sections 3.5, 3.6 and chapter 4 of the [HYSYS customization guide]



Which method do you plan to use?

Calling simulators from MATLAB

- Using ActiveX automation server
- Using native integration



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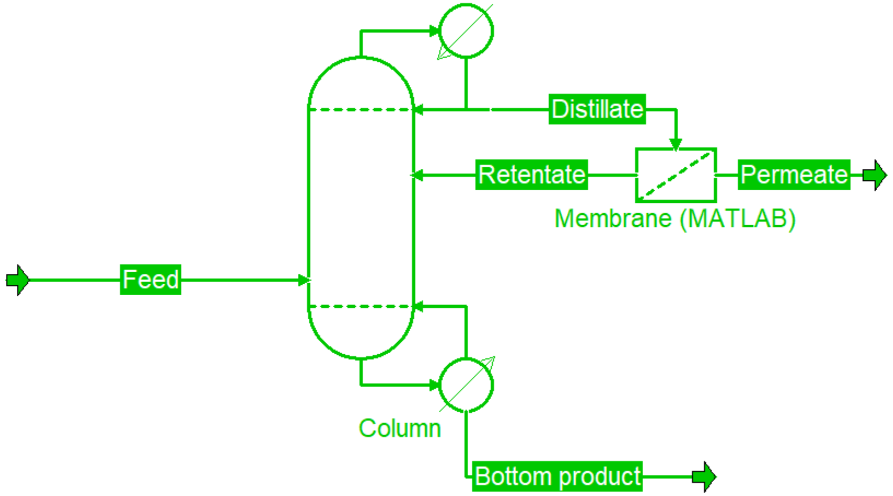

Email: Samvith.Rao@mathworks.com