



Enabling model based decision making by sharing consistent equation oriented dynamic models between multiple simulation and optimization environments

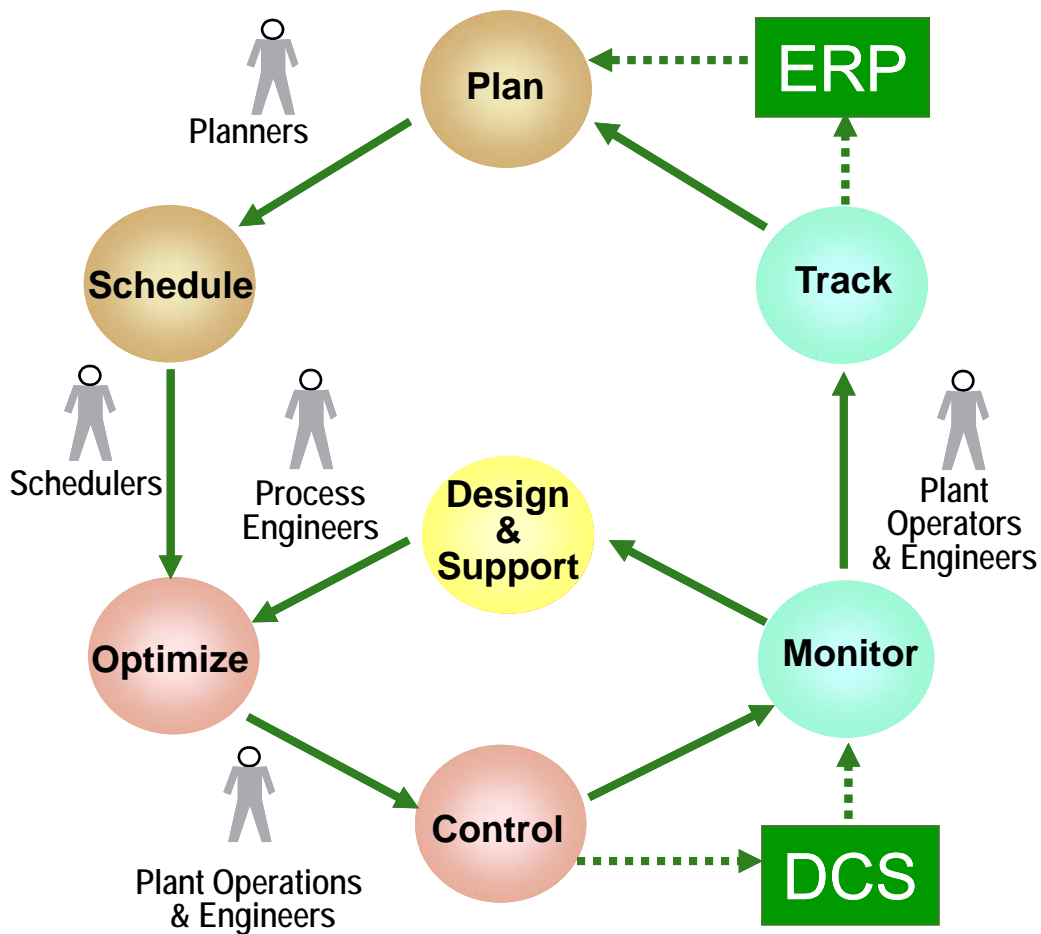
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Manager, R&D

Overview

Why do we need to use consistent models?

- How do we enable use of consistent models?
 - Common computational engine
- How do we enable consistent dynamic models?
 - Enhance common computational engine
- Sample results of the implementation
 - Dynamic batch distillation model in Aspen Plus
 - Custom dynamic tank model in Aspen HYSYS and Aspen HYSYS Dynamics

Model-Based Decision Making



Why Do We Need To Share Models?

- Consistent basis for making decisions
 - Reuse rigorous models.
- Reliability of the predictions
- Speed of deployment
- Better knowledge management
 - Standardized work process: Models created and maintained by a group; Distributed to all users
 - Lower cost. Reduces need to have experts at every site

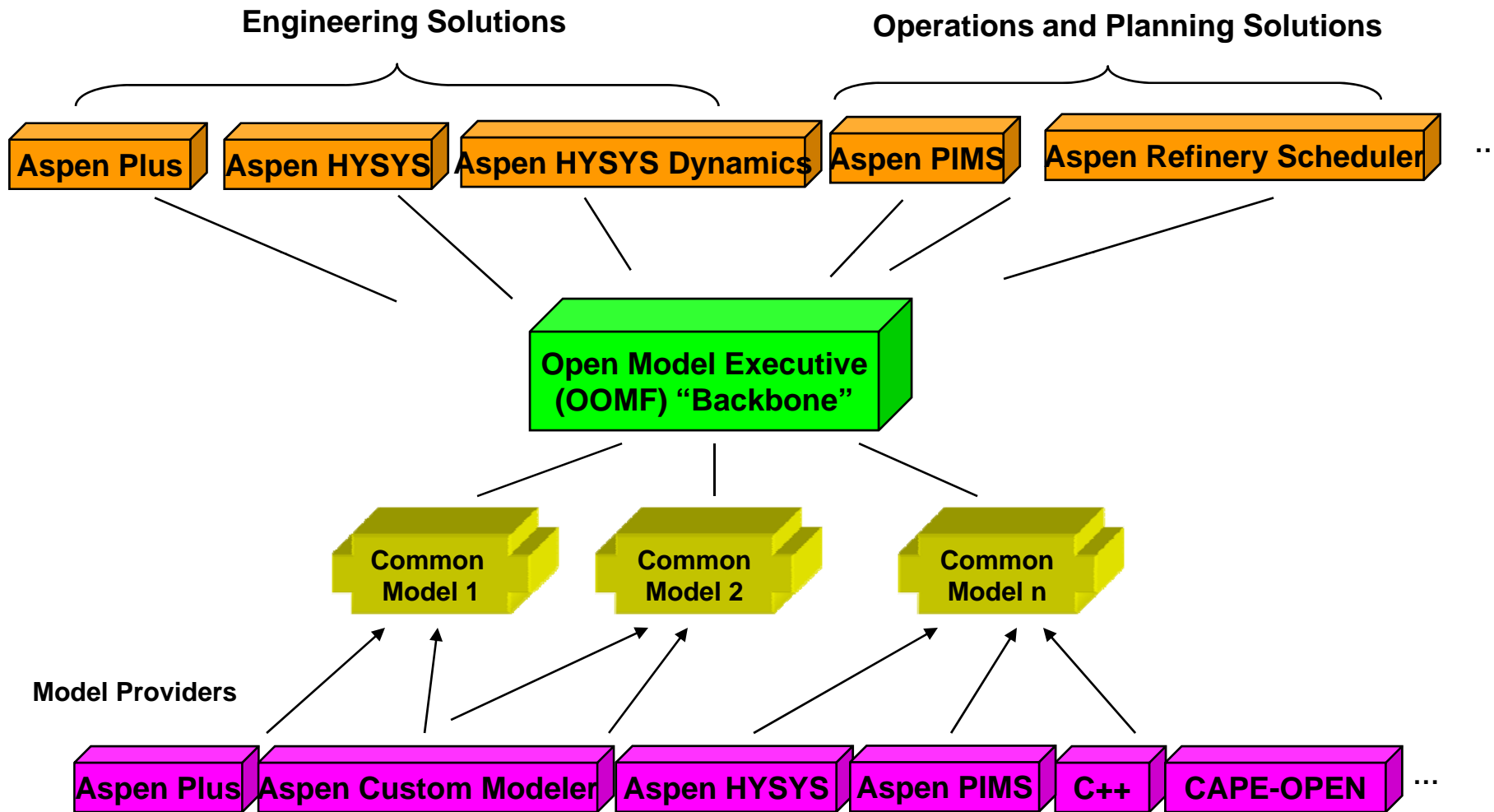
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Consistent Model-Based Decision Making Common Computational Engine



Consistent Model-Based Decision Making Common Computational Engine



Custom Steady State models can already be shared

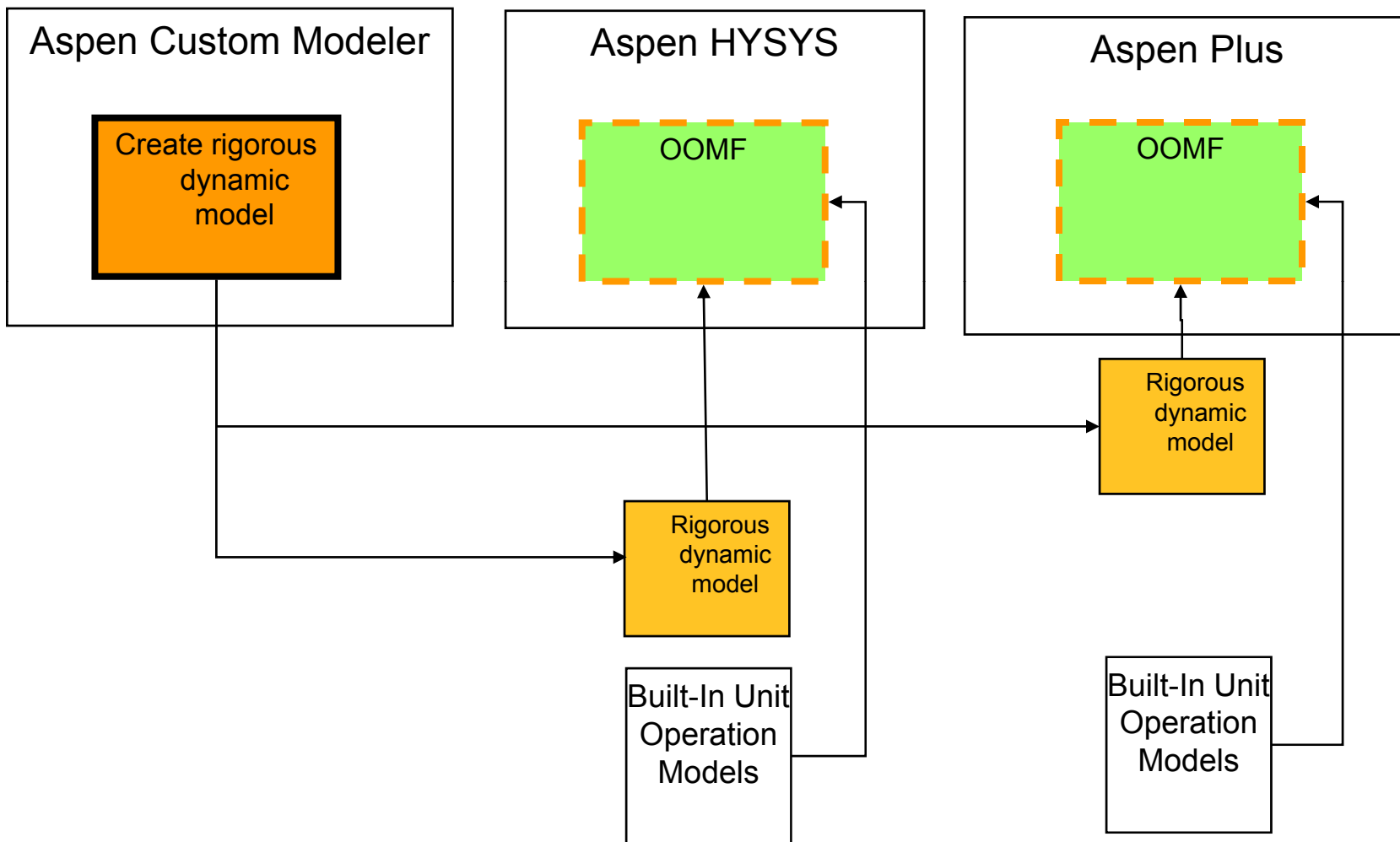
- Since 2002 steady state models developed using Aspen Custom Modeler can be seamlessly integrated into process plant models in Aspen Plus, Aspen HYSYS etc.
 - Solve in Sequential Modular and Equation Oriented solution modes
 - Icons, tables, custom forms, Visual Basic scripts are exported and available in Aspen Plus, Aspen HYSYS
 - Model variables are accessible in design specifications, sensitivity calculations, calculator blocks

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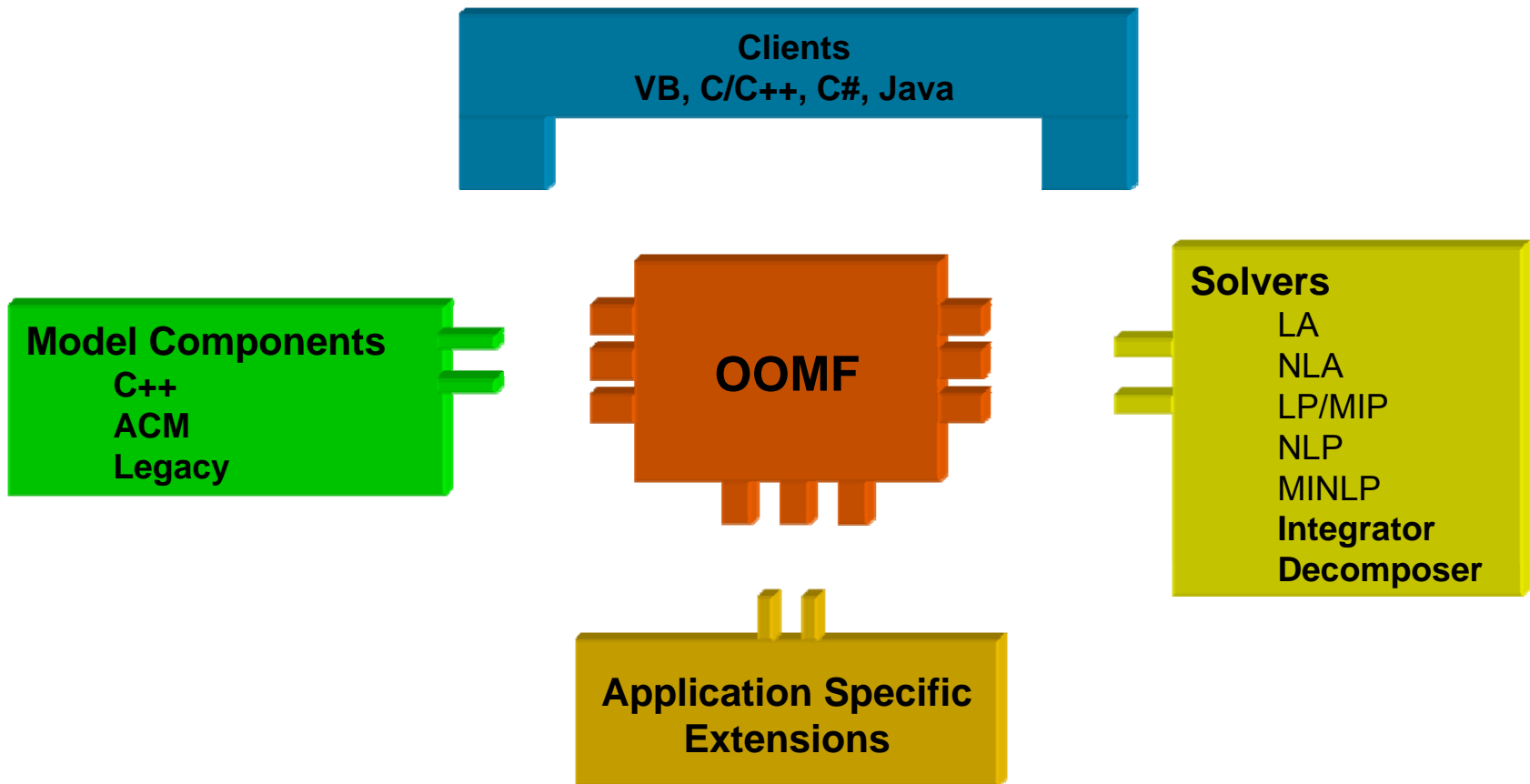
Rigorous Dynamic models can now be shared

- Author dynamic model in high level modeling environment
 - Aspen Custom Modeler
- Integrate the dynamic model with overall process model in
 - Aspen Plus and Aspen Plus Dynamics
 - Aspen HYSYS and Aspen HYSYS Dynamics
- Workflow enabled by common computational engine
 - Open Object Model Framework (OOMF)
 - Aspen Open Solvers (AOS)



Consistent Model-Based Decision Making

OOMF – Common Computational Engine

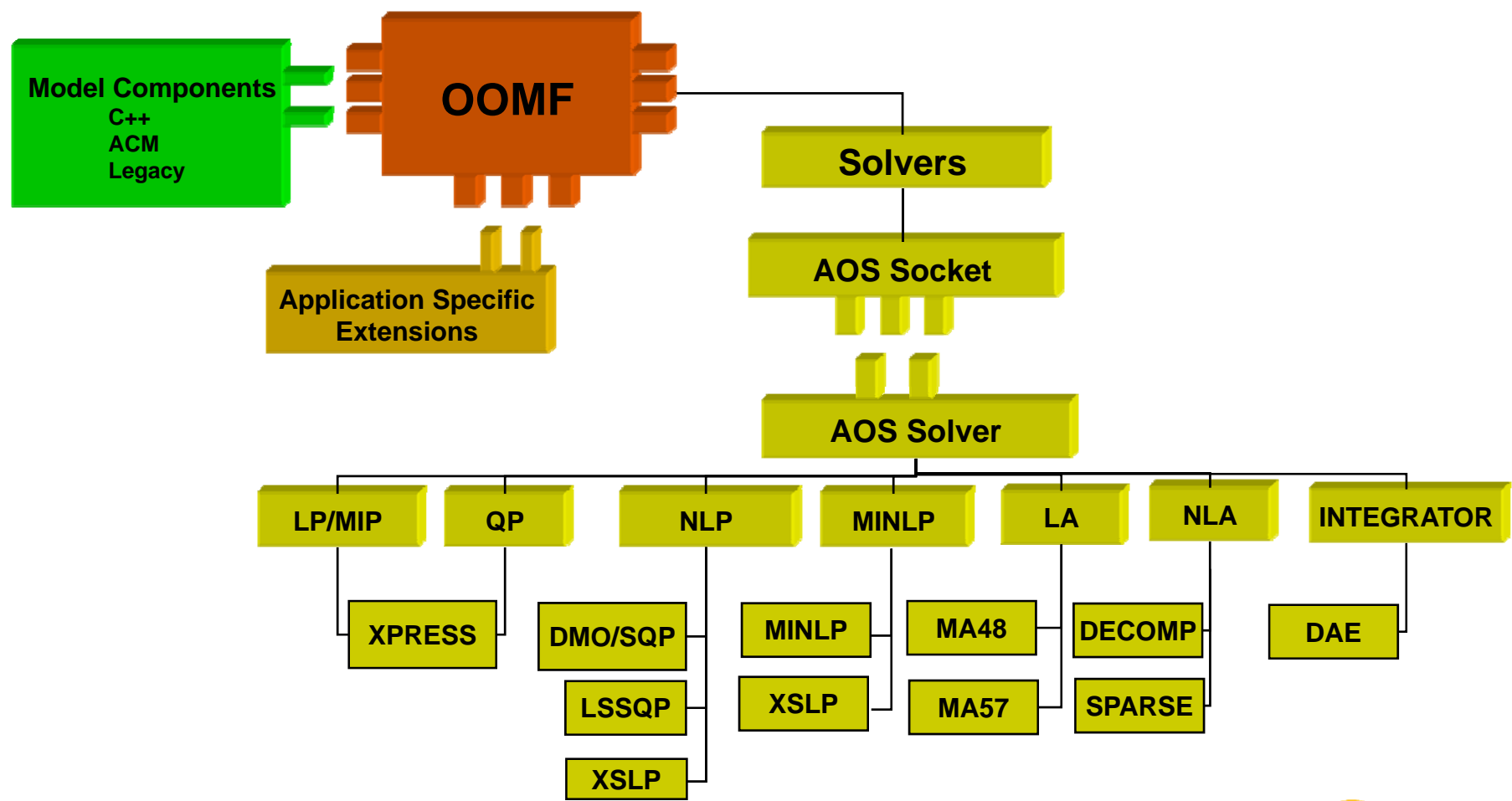


Drive the dynamic model through time

- Start, pause, re-start, and reset
- Finite State Machine
 - Manage and control the multiple states from start to end
- Task manager
 - Load, activate, parse and interpret configured tasks
- Event Manager
 - Explicit events - step the simulation through time
 - Implicit events - conditions, actions, monitors
- Data historian
 - Record, View variable time profiles; Save snapshots
- Open Solver driver
 - Differential Algebraic Equation System object

Consistent Model-Based Decision Making

Aspen Open Solvers



Solve the dynamic model

- Aspen Open Solver Integrator
 - Explicit Euler, Implicit Euler, Runge-Kutta, Gear
- Interfaces and implementation for
 - Differential Algebraic Equation System Object
 - Group Decomposition
 - Tearing
 - Homotopy
- Event location
 - Discontinuities, Tasks
- Diagnostic Reports

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Results of the implementation

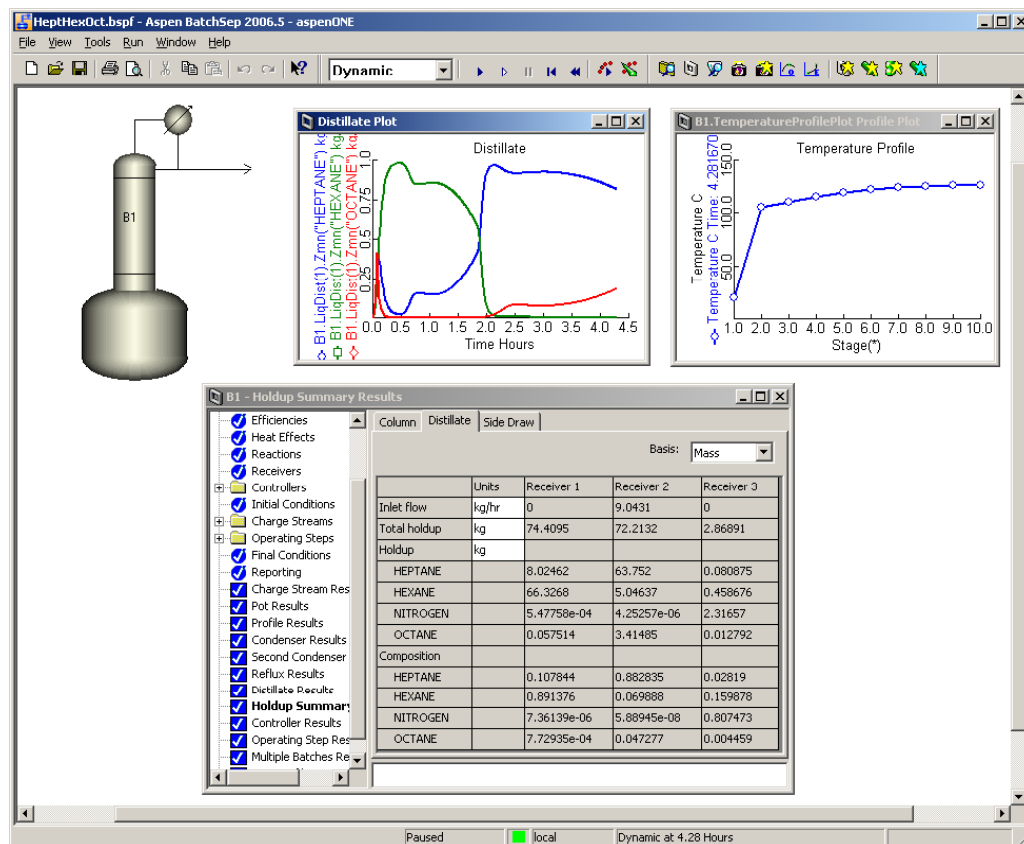
- Dynamic batch distillation model in Aspen Plus
- Custom dynamic tank model in Aspen HYSYS and Aspen HYSYS dynamics

Author the dynamic model in Aspen Custom Modeler.

- Create a dynamic model based on proprietary knowledge or chemical engineering literature
- Integrate dynamic model with overall process model in Aspen Plus and Aspen HYSYS.
- Two examples follow
 - Batch Distillation Model authored in Aspen Custom Modeler; integrated within an Aspen Plus process model
 - Custom tank model authored in Aspen Custom modeler; integrated within an Aspen HYSYS and Aspen HYSYS Dynamics model

Consistent Model-Based Decision Making Aspen Batch Distillation

- Aspen Batch Distillation is a dynamic model developed using Aspen Custom Modeler
- Used for design, analysis and optimization of batch distillation processes



- Developed using Aspen Custom Modeler
- Uses Aspen Properties
 - Rigorously model two-phase and three-phase columns
- Integrates a large DAE system
 - 1000 to 100000+ equations
 - Implicit Euler or Gear solution methods
- Uses tasks to model a sequence of batch operations
- Rich user interface for configuring column and operating steps

Consistent Model-Based Decision Making Aspen Batch Distillation Sample Model

• Water-methanol separation

basic_setup_answer.bspf - Aspen Batch Distillation V7.0 - aspenONE

File Edit View Tools Flowsheet Run Window Special Help

Dynamic

Process Flowsheet Window

B1

B1 - Profile Results

- Setup
- Jacket Heating
- Pressure/Holdups
- Internals
- Efficiencies
- Heat Effects
- Reactions
- Receivers
- Controllers
- Initial Conditions
- Charge Streams
- Operating Steps
- Final Conditions
- Reporting
- Charge Stream Res
- Pot Results
- Profile Results**
- Condenser Results
- Second Condenser
- Reflux Results
- Distillate Results
- Holdup Summary R

TPFQ Composition Holdup Reactions Properties Flooding

Current profiles

Profiles at end of operating step

Basis: Mole

Stage	Temperature C	Pressure bar	Heat duty GJ/hr	Liquid flow kmol/hr	Vapor flow kmol/hr
Drum	67.0956	1.01325	0	14.245	0
Condenser	69.3064	1.01325	-0.548219	9.74499	0
2	76.8348	1.02436	0	8.07164	14.8037
3	91.6797	1.03547	0	6.37879	13.96
4	98.1496	1.04658	0	5.8302	13.1916
5	99.2283	1.05769	0	5.62957	13.0832
6	99.6317	1.06881	0	5.54059	13.0754
7	99.9759	1.07992	0	5.49215	13.078

Comp Profile Plot

METHANOL kmol/kmol Time: 1.487805

WATER kmol/kmol Time: 1.487805

B1.TemperatureProfilePlot Profile Plot

Temperature C Time: 1.487805

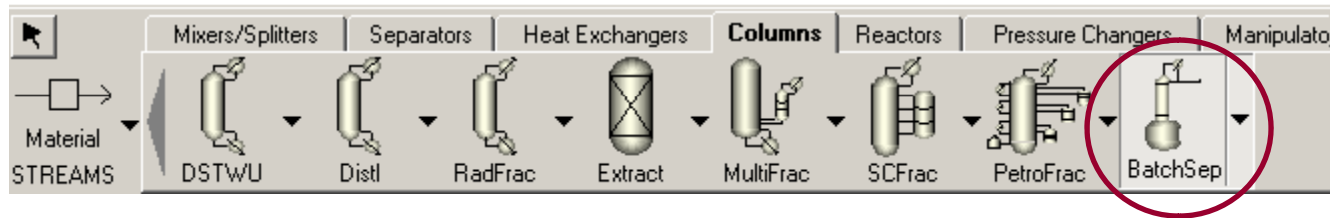
BatchSep Models SubModels

STREAMS Connection BatchSep Hierarchy

Ready Paused local Dynamic at 1.49 Hours

Consistent Model-Based Decision Making Integration into Aspen Plus Via OOMF

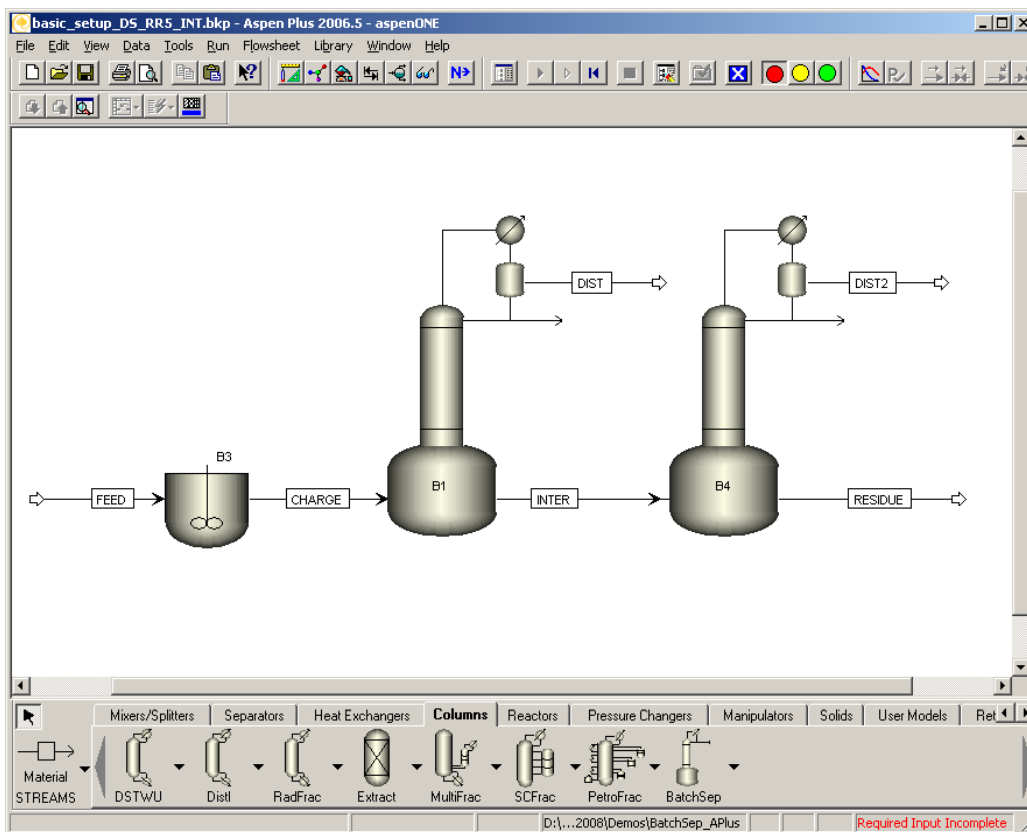
- Aspen Batch Distillation Model now also available as a unit operation in Aspen Plus



- Integration with Aspen Plus enables simulation and optimization of:
 - Batch distillation sequences
 - Entire process including other batch or continuous unit operations

Consistent Model-Based Decision Making Integration into Aspen Plus Via OOMF

- Connect to other models and optimize the process
 - Notional buffer tanks at inlets and outlets



Consistent Model-Based Decision Making Integration into Aspen Plus Via OOMF

• Water-methanol separation using Aspen Plus

basic_setup_answer_str.bkp - Aspen Plus V7.0 - aspenONE

File Edit View Data Tools Run Library Window Costing Help

Process Flowsheet Window

Block B1 (BatchSep) - Data Browser

Block B1 (BatchSep) - Plot

Block B1 (BatchSep) - Plot

Mixers/Splitters Separators Heat Exchangers Columns Reactors Pressure Changers Manipulators Solids User Models Retired Models

Materials: DSTWU, Distl, RadFrac, Extract, MultiFrac, SCFrac, PetroFrac, BatchSep

For Help, press F1

D:\AICHE Results Available

Block B1 (BatchSep) - Data Browser

TPFQ | Composition | Holdup | Properties | Flooding

Current profiles

Profiles at end of operating step

Basis: Mole

Stage	Temperature C	Pressure BAR	Heat duty GCAL/HR	Liquid flow KMOL/HR	Vapor flow KMOL/HR
Drum	67.1463	1.01325	0	14.2596	0
Condenser	69.2954	1.01325	-0.131626	9.75956	0
2	76.8608	1.02436	0	7.99825	14.8227
3	91.7748	1.03547	0	6.34508	13.9072
4	98.1759	1.04658	0	5.81776	13.176
5	99.2387	1.05769	0	5.62257	13.0832
6	99.6405	1.06881	0	5.53568	13.0771
7	99.9845	1.07992	0	5.48786	13.0796

Block B1 (BatchSep) - Plot

Block B1 (BatchSep)

METHANOL

WATER

Stage

Block B1 (BatchSep) - Plot

Block B1 (BatchSep)

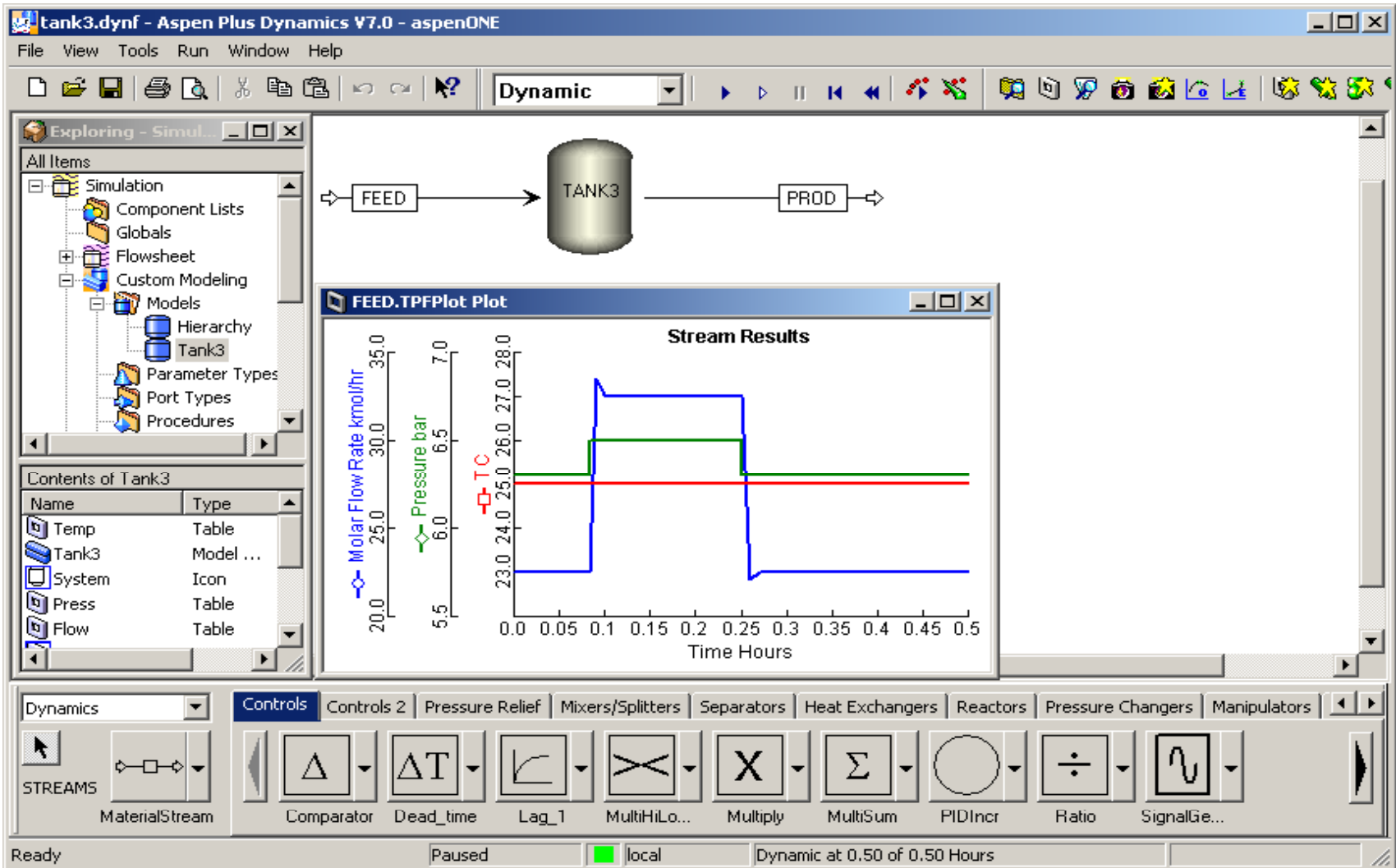
Temperature C

Stage

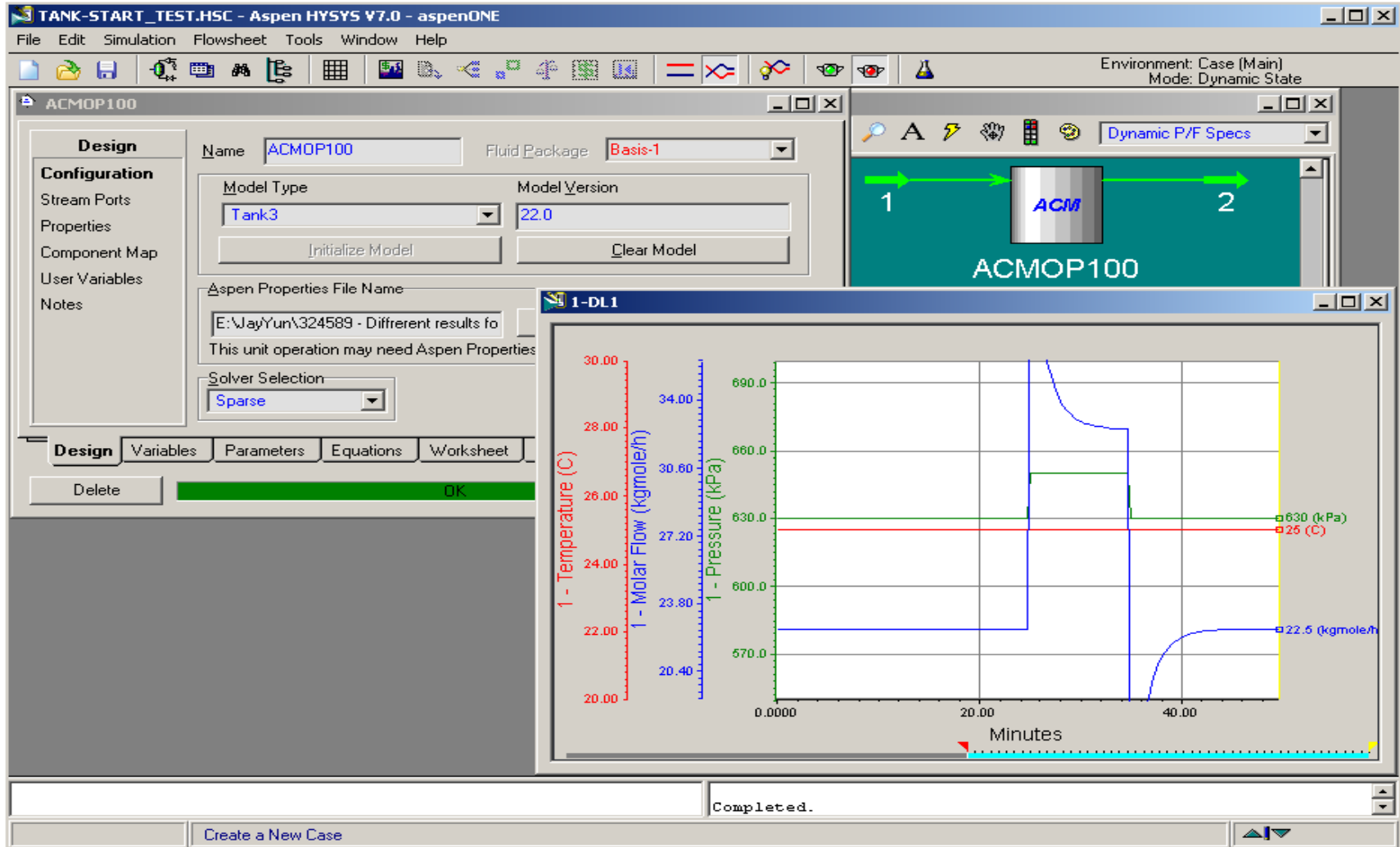
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Consistent Model-Based Decision Making Custom Dynamic Tank Model



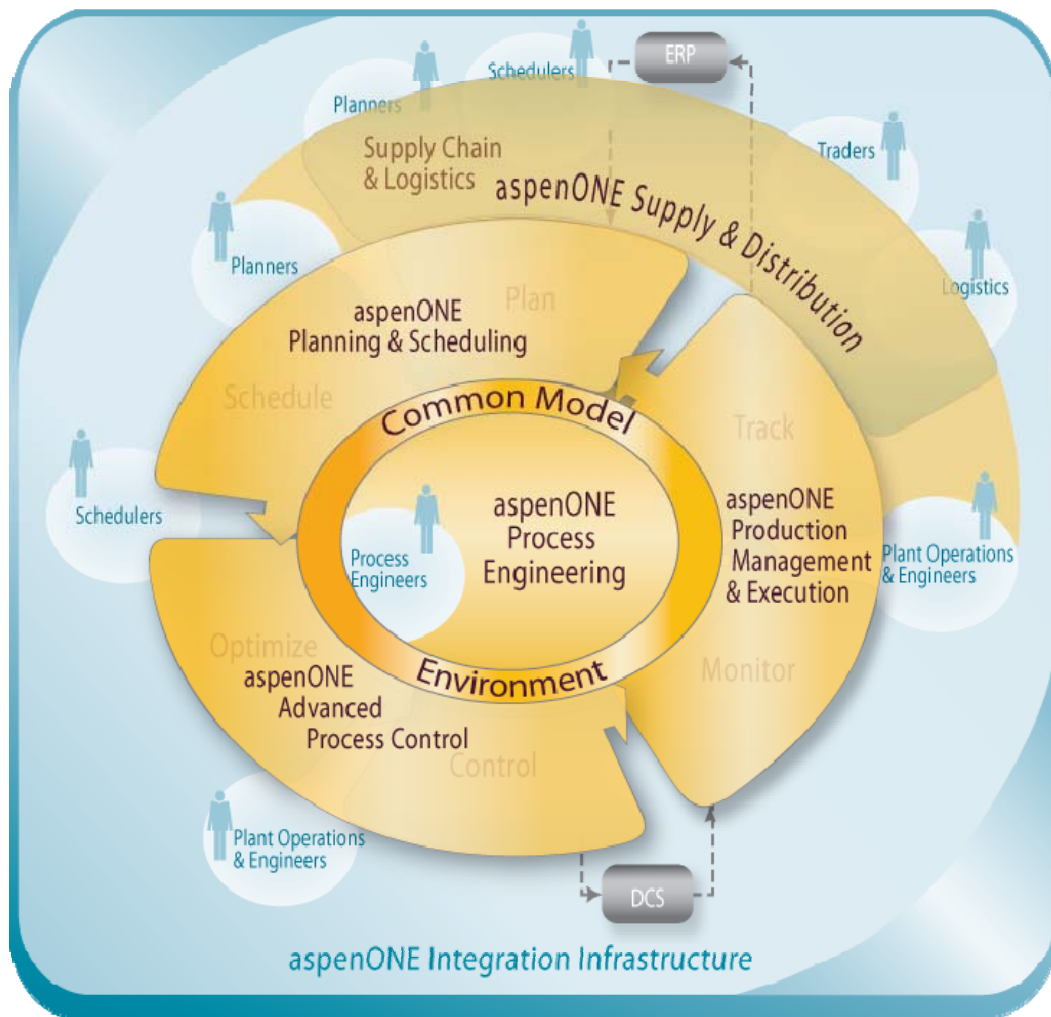
Consistent Model-Based Decision Making Integration into Aspen HYSYS Via OOMF



Dynamic models can be shared for better decision making.

- Author dynamic model in high level modeling environment
 - Aspen Custom Modeler
- Integrate the dynamic model with overall process model
 - Aspen Plus and Aspen Plus Dynamics
 - Aspen HYSYS and Aspen HYSYS Dynamics
- Improve process model accuracy, reliability and deployment.
 - Better knowledge management
- Workflow enabled by common computational engine
 - Open Object Model Framework (OOMF)
 - Aspen Open Solvers (AOS)

Consistent Model-Based Decision Making



- **Common Model Environment**
 - Enables use of consistent models in Engineering, Planning and Scheduling, Advanced Control, Optimization, and Operations
- Sample implementations of sharing of dynamic model in engineering were described in this paper.
 - The next paper will describe how similar models are used across Engineering, Planning and Scheduling, and Operations in the refining industry

Acknowledgements

- Ashok Bhakta
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- Ajay Modi
- James Goom