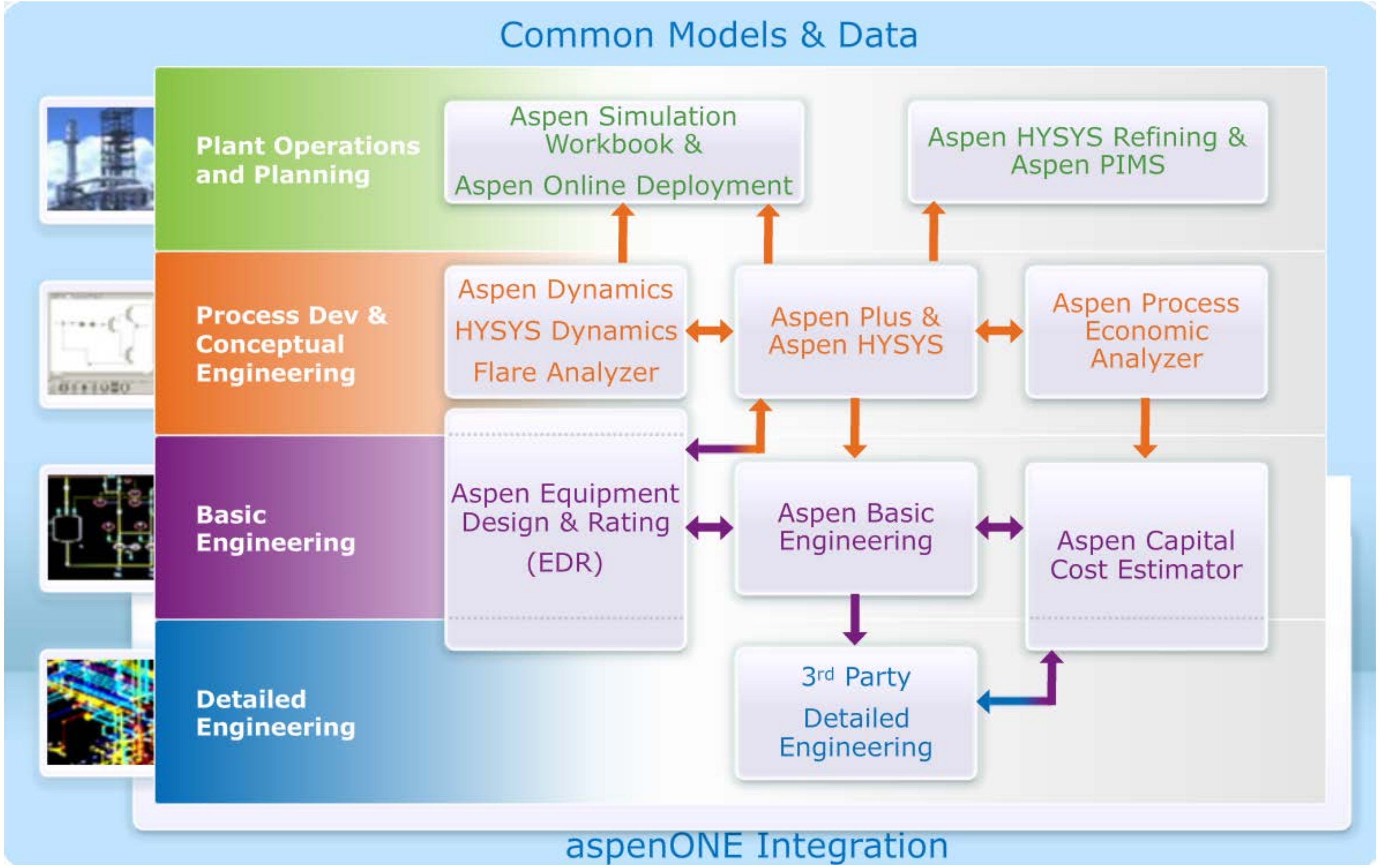
ASPEN ENGINEERING SUITE OVERVIEW

General Overview

Software for integrated process engineering, including steady-state and dynamic process simulation, equipment design, and cost evaluation.



Source: Aspen Technology, 2012

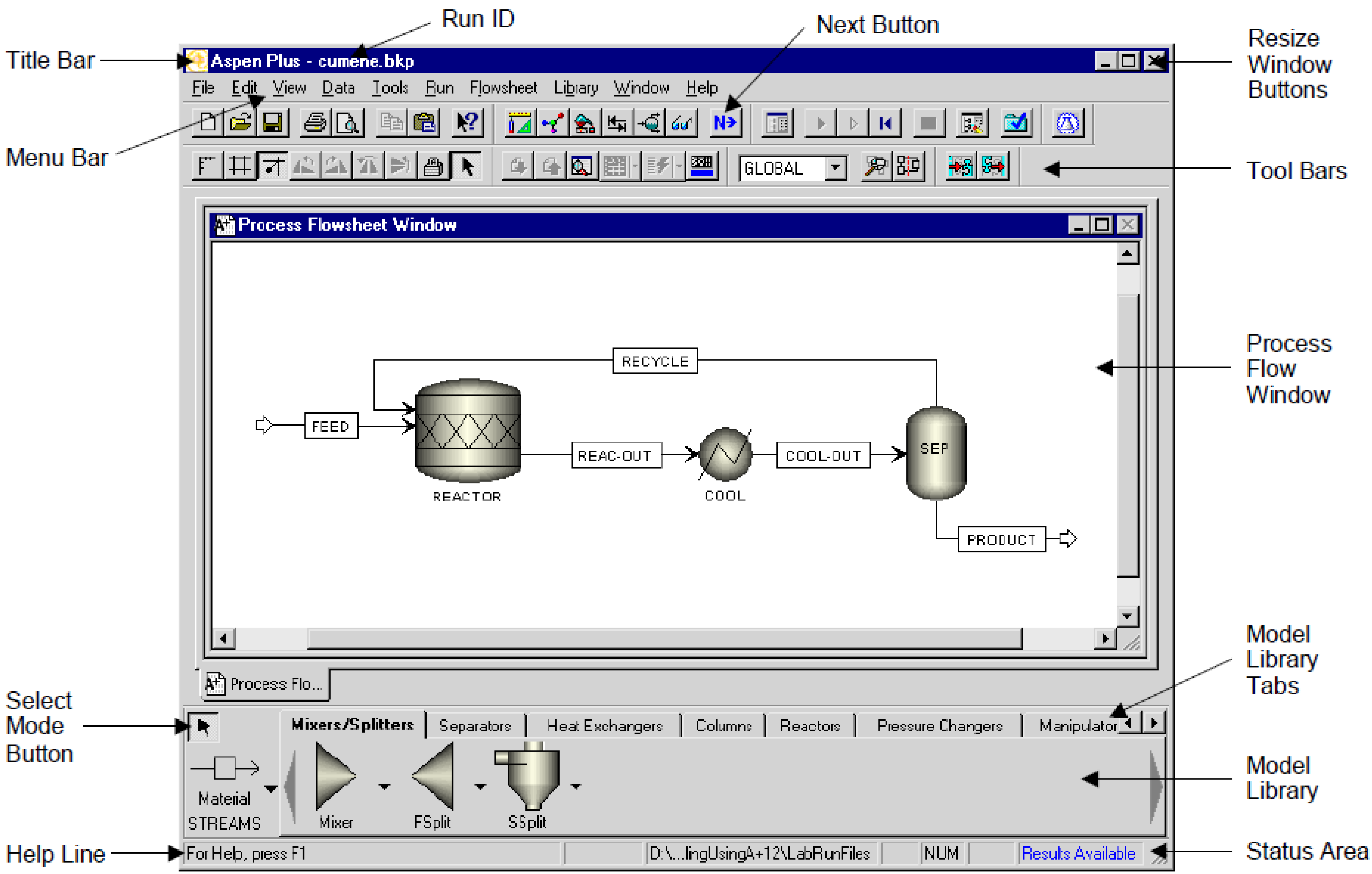
ASPEN PLUS

OVERVIEW

Aspen Plus

- Aspen Plus is a process modeling tool for conceptual design, optimization, and performance monitoring for diverse industries. Aspen Plus is a core element of AspenTech's Process Engineering applications.
- Given thermodynamic data, realistic operating conditions, and rigorous equipment models➔ Its possible to simulate actual plant behaviors, by using **basic engineering relations such as mass and energy balances, and phase and chemical equilibrium**
- **Features**
  - ➢ Best-in-class physical properties methods and data
  - ➢ Diverse Model library : Simulation of a wide range of processes
  - ➢ Scalability for large and complex processes
  - ➢ Online deployment of models: real-time optimization/advanced process control applications
  - ➢ Workflow automation: Aspen Plus models can be linked to Microsoft Excel® using Aspen Simulation Workbook or Visual Basic®

Aspen Plus



Source: Aspen Technology, 2012

Simulation Steps

1. Define Process Flow Sheet.
   Units –Streams-Models

2. Specify Chemical Components

3. Specify Thermodynamic Model
   Estimation of physical properties

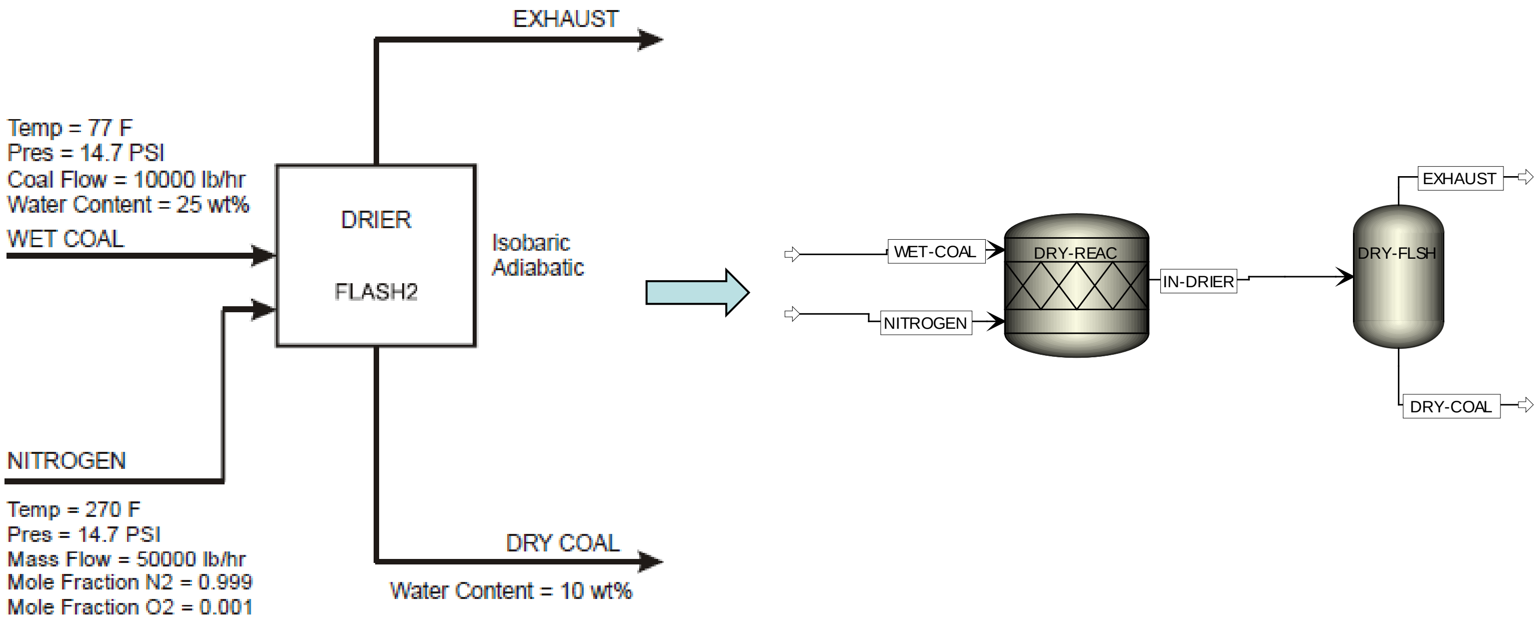
4. Specify Flow Rates and Thermodynamic conditions

5. Run Simulation – Analyze Results

Example

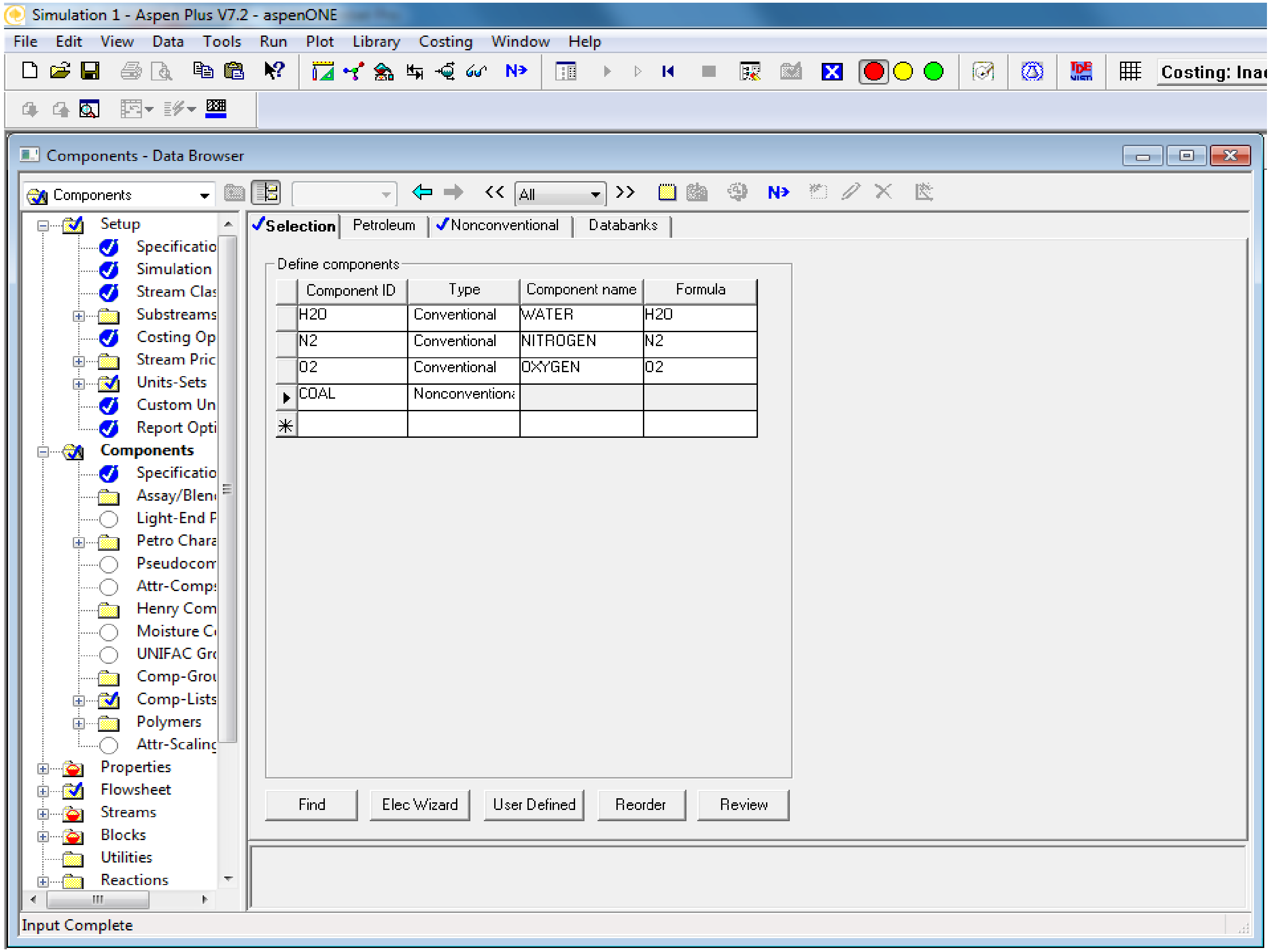
Define Process Flow Sheet

Coal Drying Flowsheet



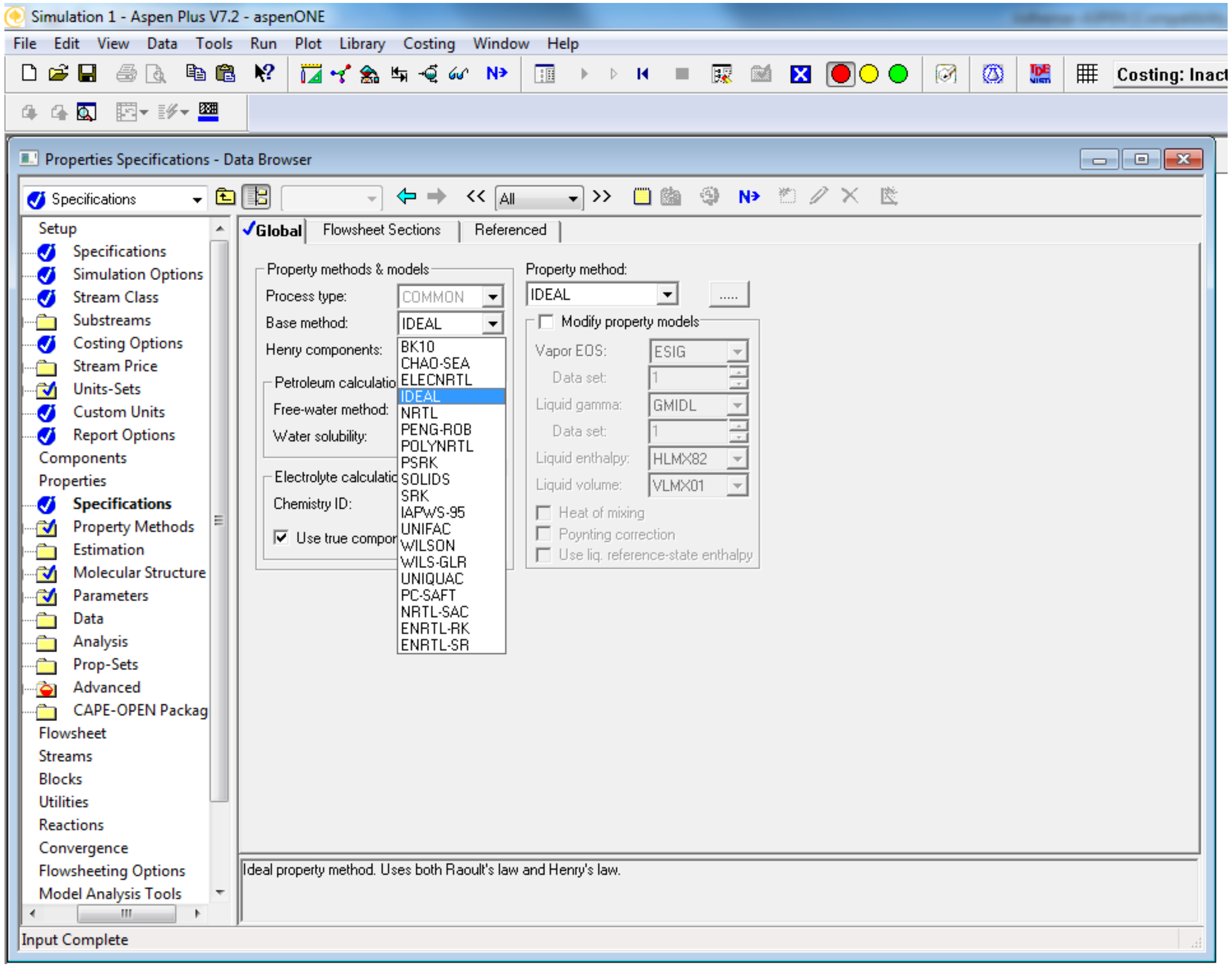
Source: Aspen Technology, 2012

Specify Chemical Components



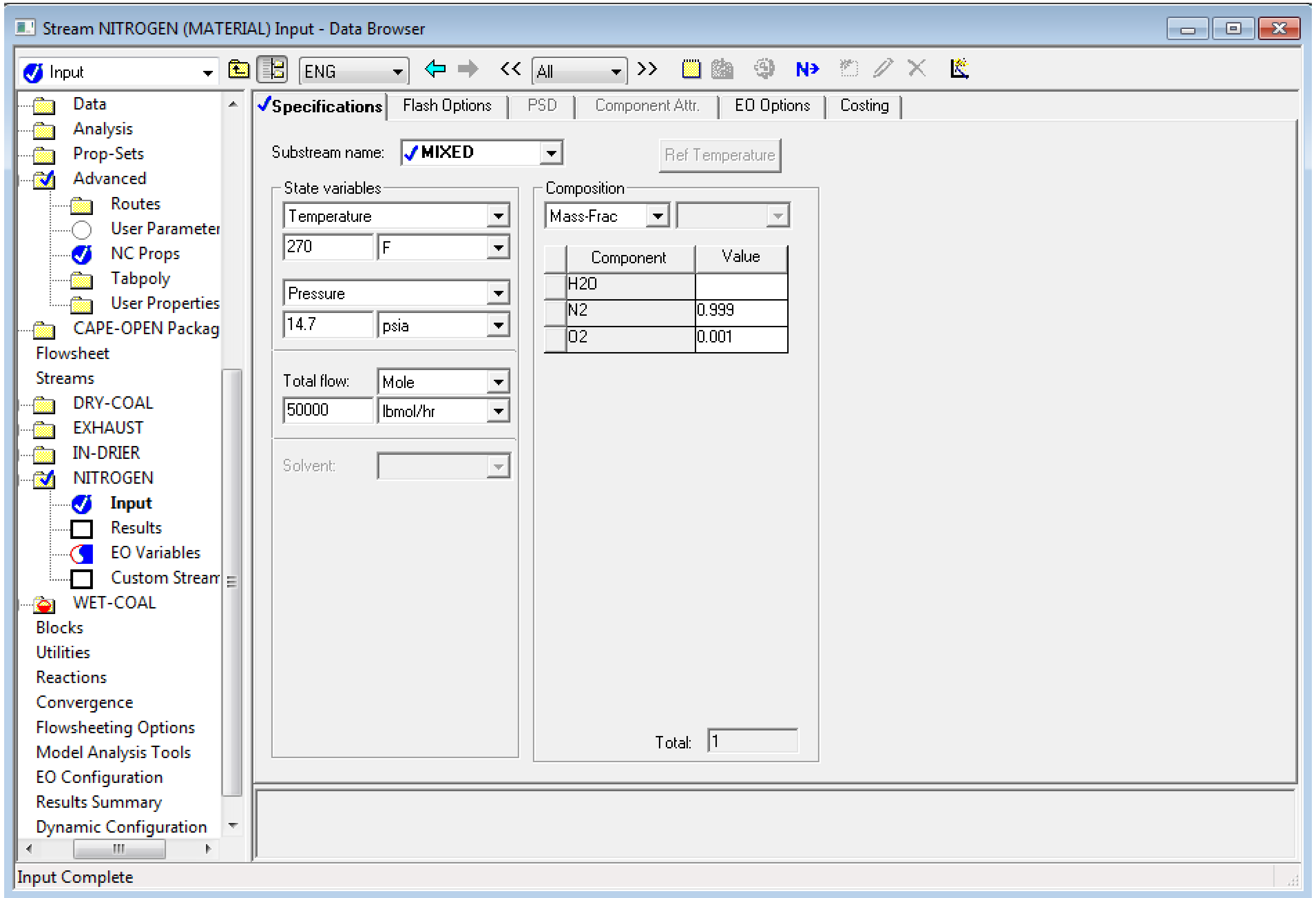
Source: Aspen Technology, 2012

Specify Thermodynamic Model



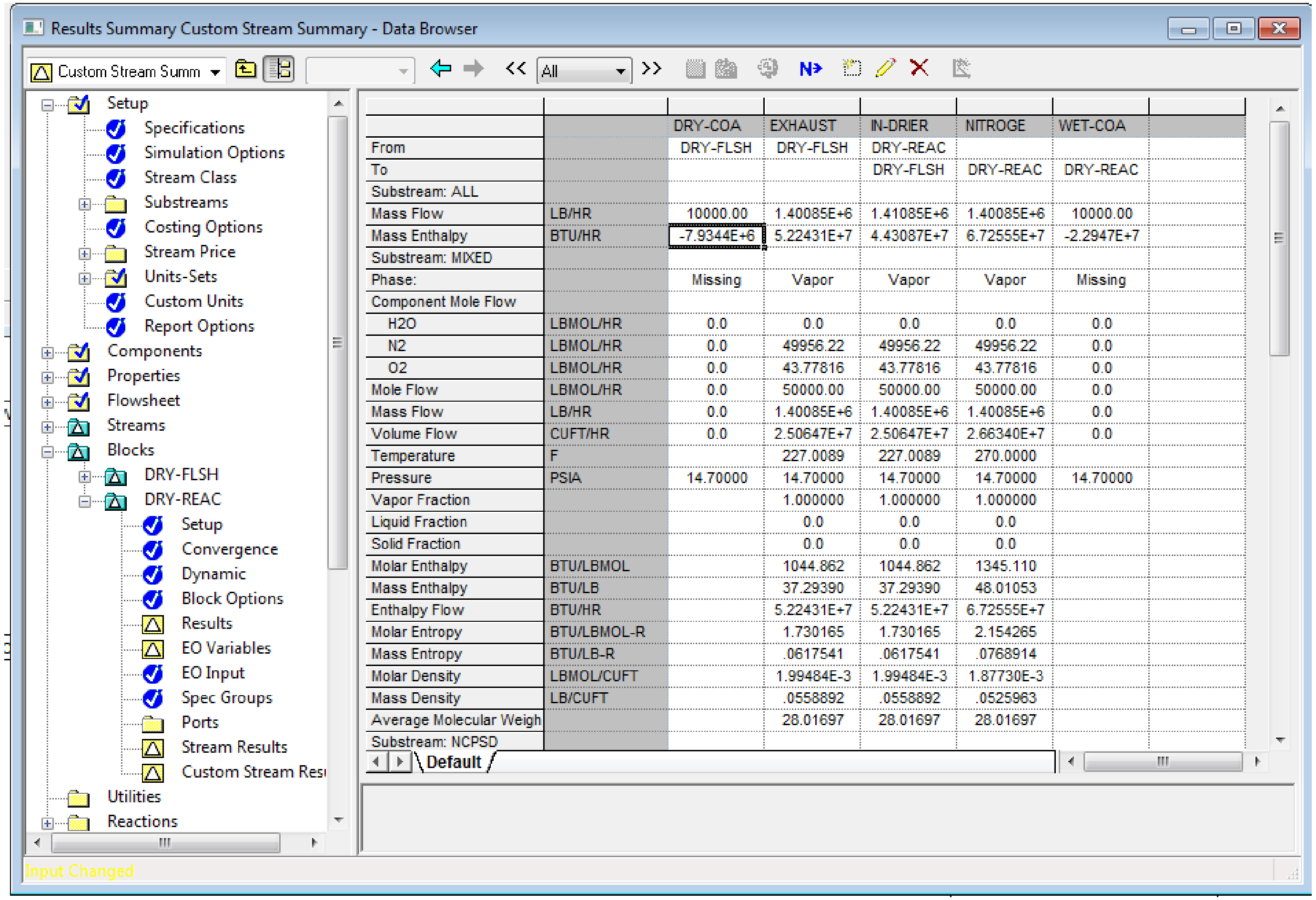
Source: Aspen Technology, 2012

Specify Flow Rates conditions



Source: Aspen Technology, 2012

Simulation Results



		DRY-COA	EXHAUST	IN-DRIER	NITROGE	WET-COA
From		DRY-FLSH	DRY-FLSH	DRY-REAC		
To				DRY-FLSH	DRY-REAC	DRY-REAC
Substream: ALL						
Mass Flow	LB/HR	10000.00	1.40085E+6	1.41085E+6	1.40085E+6	10000.00
Mass Enthalpy	BTU/HR	-7.9344E+6	5.22431E+7	4.43087E+7	6.72555E+7	-2.2947E+7
Substream: MIXED						
Phase:		Missing	Vapor	Vapor	Vapor	Missing
Component Mole Flow						
H2O	LBMOL/HR	0.0	0.0	0.0	0.0	0.0
N2	LBMOL/HR	0.0	49956.22	49956.22	49956.22	0.0
O2	LBMOL/HR	0.0	43.77816	43.77816	43.77816	0.0
Mole Flow	LBMOL/HR	0.0	50000.00	50000.00	50000.00	0.0
Mass Flow	LB/HR	0.0	1.40085E+6	1.40085E+6	1.40085E+6	0.0
Volume Flow	CUFT/HR	0.0	2.50647E+7	2.50647E+7	2.66340E+7	0.0
Temperature	F		227.0089	227.0089	270.0000	
Pressure	PSIA	14.70000	14.70000	14.70000	14.70000	14.70000
Vapor Fraction			1.000000	1.000000	1.000000	
Liquid Fraction			0.0	0.0	0.0	
Solid Fraction			0.0	0.0	0.0	
Molar Enthalpy	BTU/LBMOL		1044.862	1044.862	1345.110	
Mass Enthalpy	BTU/LB		37.29390	37.29390	48.01053	
Enthalpy Flow	BTU/HR		5.22431E+7	5.22431E+7	6.72555E+7	
Molar Entropy	BTU/LBMOL-R		1.730165	1.730165	2.154265	
Mass Entropy	BTU/LB-R		.0617541	.0617541	.0768914	
Molar Density	LBMOL/CUFT		1.99484E-3	1.99484E-3	1.87730E-3	
Mass Density	LB/CUFT		.0558892	.0558892	.0525963	
Average Molecular Weigh			28.01697	28.01697	28.01697	
Substream: NCPSD						

Source: Aspen Technology, 2012

ASPEN CUSTOM MODELER

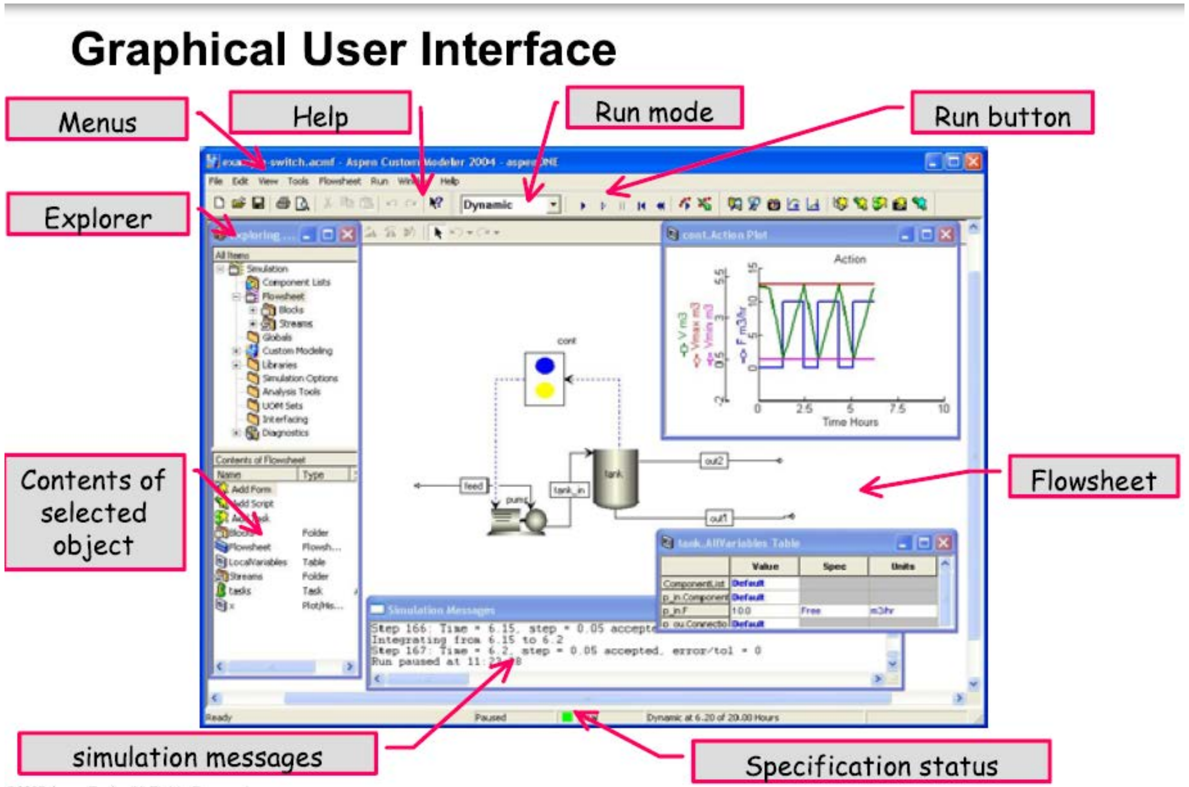
OVERVIEW

General Overview

- Aspen Custom Modeler is a process and equipment model development and simulation environment
- Aspen Custom Modeler (ACM) is used to **create** rigorous models of processing equipment and to apply these equipment models to simulate and optimize continuous, batch, and semi-batch processes.
- It is used across many industries including chemicals, power, nuclear, food and beverage, metals and minerals, pharmaceuticals, and othrers

Features

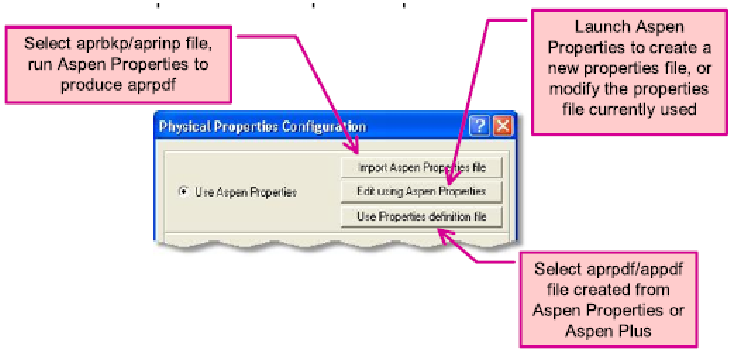
Designed for process engineers : ACM uses a flow sheeting environment based on streams and equipment and includes built-in understanding of components and process thermodynamics.

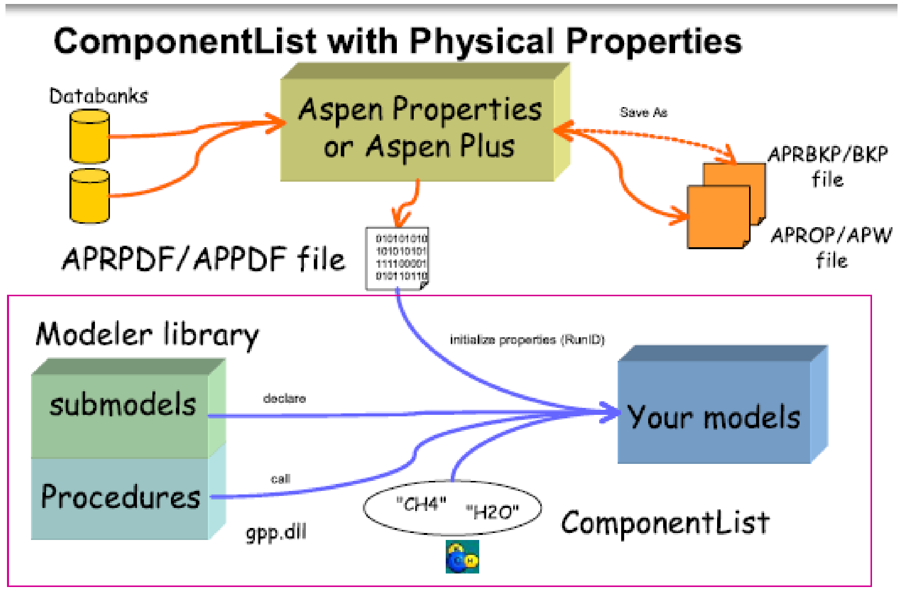


Source: Aspen Technology, 2012

Features

Physical properties methods and data: ACM is fully integrated with Aspen Properties, it includes extensive databases of pure component and phase equilibrium data for chemicals, electrolytes, solids, and polymers





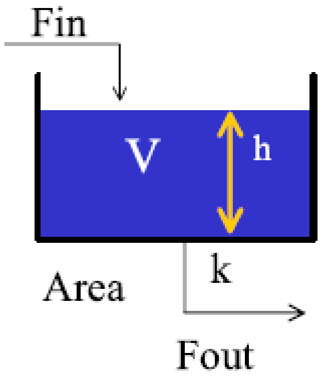
Source: Aspen Technology, 2012

Features

Equation oriented architecture : ACM language is **declarative**, you say **"what"** you want and leave it to ACM to find out **"how".**

- Solver for system of **Algebraic Equations**, based on Newton iterative procedure

• Steady State model: 3 equations, 6 variables



Equations

$$0 = F_{in} - F_{out}$$

$$F_{out} = k.\sqrt{h}$$

$$V = A.h$$

ACM language

```
Fin, Fout as flow_vol;
k as realvariable;
h as length;
V as volume;
A as area;

0    = Fin - Fout;
Fout = k*sqrt(h);
V    = A*h;
```

B1.AllVariables Table

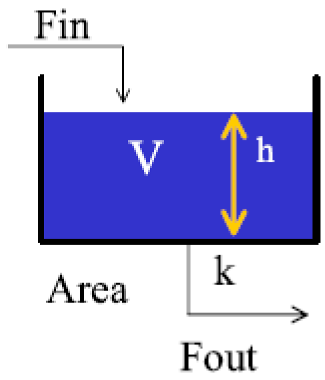
	Value	Spec	Units
A	1.0	Fixed	m2
ComponentList	Default		
Fi	1.0	Fixed	m3/hr
Fo	1.0	Free	m3/hr
h	1.0	Free	m
k	1.0	Fixed	
V	10.0	Free	m3

Note that the equations need not be variable = expression, they can be expression = another expression

Source: Aspen Technology, 2012

Features

- System of **differential and algebraic equations**



Equations

accumulation

$$\frac{dV}{dt} = F_{in} - F_{out}$$

$$F_{out} = k.\sqrt{h}$$

$$V = A.h$$

```
Fin, Fout as flow_vol;
k as realvariable;
h as length;
V as volume;
A as area;

$V    = Fin - Fout;
Fout = k*sqrt(h);
V     = A*h;
```

Variable	type	specification
Fin	algebraic	FIXED
Fout	algebraic	FREE
V	state	FREE
k	algebraic	FIXED
h	algebraic	INITIAL
A	algebraic	FIXED

$variable in ACM language represents the time derivative of the variable

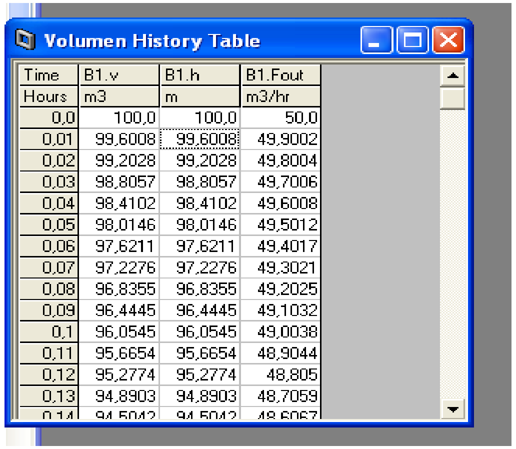
Source: Aspen Technology, 2012

Integration Algorithms

- Implicit: Implicit Euler (fixed or variable step), gear
- Explicit: Explicit Euler, Runge Kutta

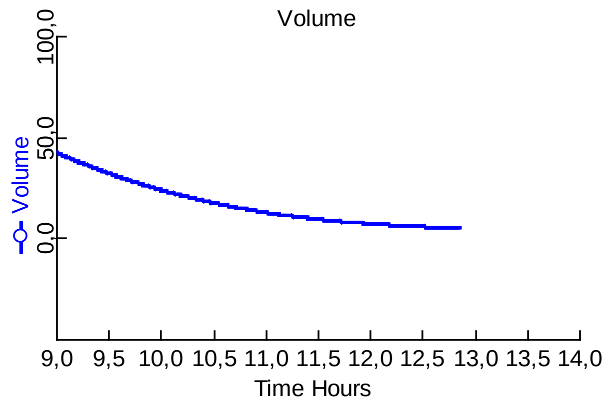
Features

Flexible user-defined forms

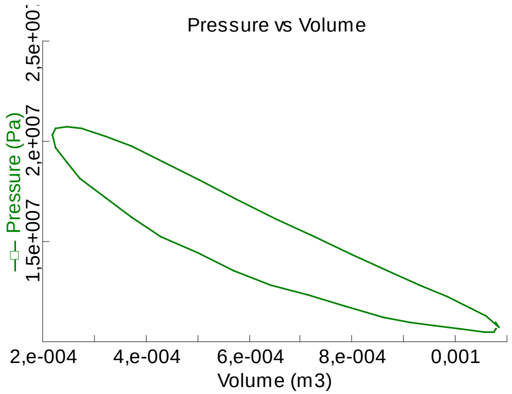

Volumen History Table

Time	B1.v	B1.h	B1.Fout
Hours	m3	m	m3/hr
0,0	100,0	100,0	50,0
0,01	99,6008	99,6008	49,9002
0,02	99,2028	99,2028	49,8004
0,03	98,8057	98,8057	49,7006
0,04	98,4102	98,4102	49,6008
0,05	98,0146	98,0146	49,5012
0,06	97,6211	97,6211	49,4017
0,07	97,2276	97,2276	49,3021
0,08	96,8355	96,8355	49,2025
0,09	96,4445	96,4445	49,1032
0,1	96,0545	96,0545	49,0038
0,11	95,6654	95,6654	48,9044
0,12	95,2774	95,2774	48,805
0,13	94,8903	94,8903	48,7059
0,14	94,5042	94,5042	48,6067

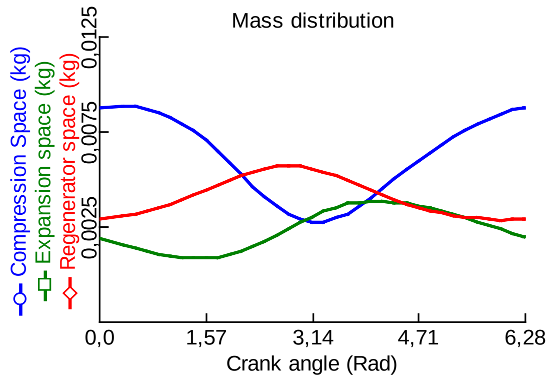
Table Forms



Time series Plot forms



Phase Plots

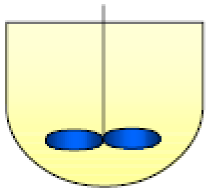


Profile Plots

Features

- **Optimization and estimation tools** enabling parameter fitting, data reconciliation, and steady-state and dynamic process optimization.

Estimation example

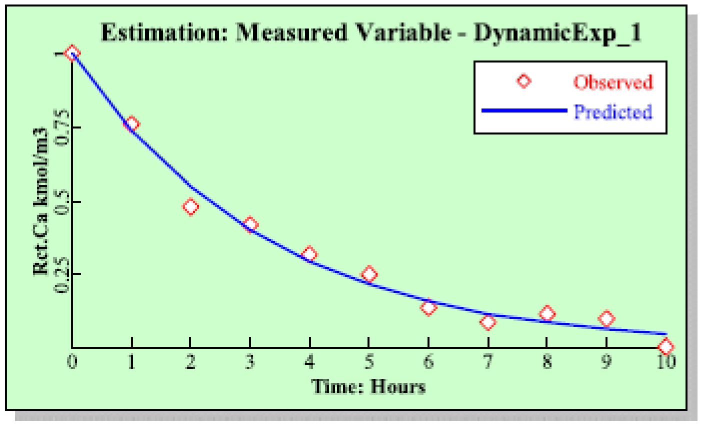


$$r = k_0 . e^{-E/RT} . C_A^{\ a}$$

$$dC_A/dt = -r$$

$$dC_B/dt = r$$

k0 = 9.74 (standard deviation 0.39)



Source: Aspen Technology, 2012

The model is fitted by finding the best values for the adjustable parameters (fixed variables)

Optimization example

Dynamic Optimization

$$\min \quad g(\dot{x}(t_f), x(t_f), z(t_f), u(t), v)$$

Objective

Minimize cost;
Maximize production;
Final time;
Batch time;
Grade transition time

subject to

$$\left.\begin{array}{l} F(\dot{x}, x, z, \theta) = 0 \\ x = x(t),\ x(0) = x_0 \\ L(i) \le x(i) \le U(i) \end{array}\right\} \text{DAE}$$

$$0 \le t \le t_f$$

$$\left.\begin{array}{l} C(\dot{x}(t_f), x(t_f), z(t_f)) = 0 \\ C(\dot{x}(t_f), x(t_f), z(t_f)) \ge 0 \end{array}\right\} \text{Constraints}$$

Maximum reactor temperature over time;
Final concentration of components

$$L(i) \le \{u_i(t), v(i)\} \le U(i)$$

Decision and control variables

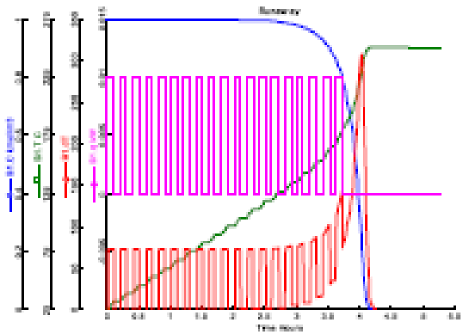
Initial concentrations;
Model parameters;
Control functions;
Final time;
Reaction rates;
Reflux ratios

Features

- **Flexible Task Language** to define batch recipes, transition schemes, or to simulate process equipment failures or other disturbances

Heating System example:

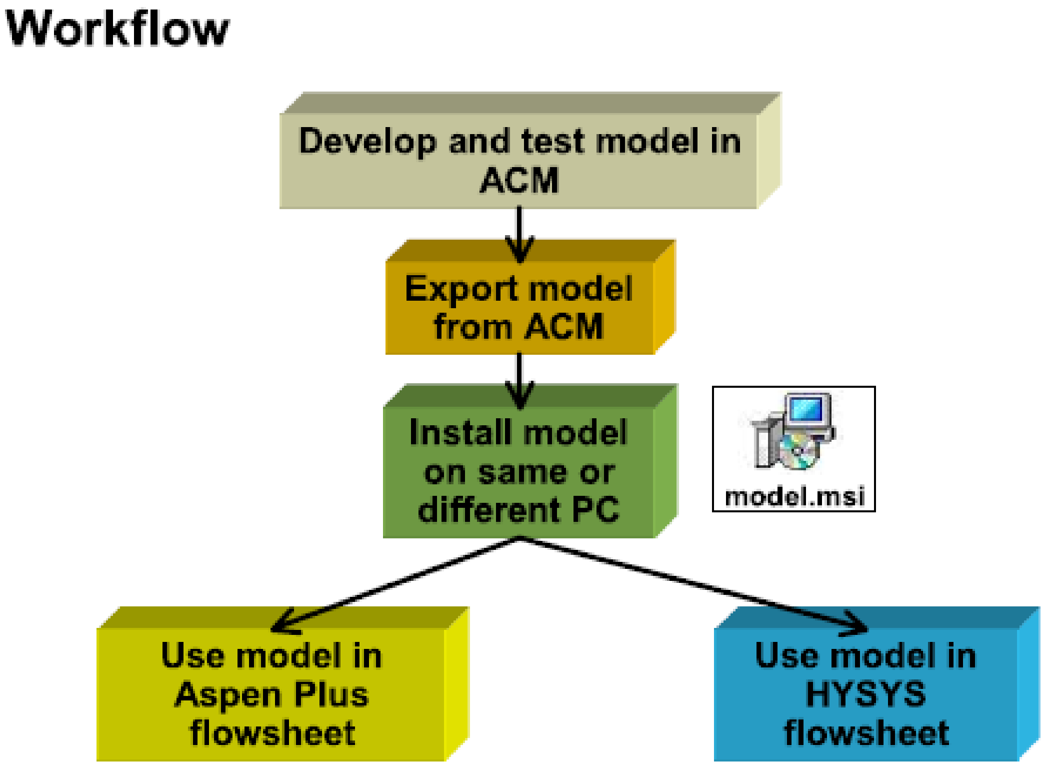
```
Task hw runs at 0.01
  while B1.dT < 100 do
    B1.q : 0.01 {kW}; // heat
    wait 0.1;
    B1.q : 0; // stop heat
    wait 0.1;
  endwhile;
End
```



Source: Aspen Technology, 2012

Features

- **Export Equipments or process models**



Source: Aspen Technology, 2012

Features

•**Library of control models :** to simulate process control systems.

•**Online deployment of models :** ACM includes an OLE for Process Control (OPC) interface, enabling links to process control and information management systems

•**Workflow automation**: ACM models can be linked to Microsoft Excel® using Aspen Simulation Workbook or Visual Basic®, enabling workflow automation and allowing model deployment to casual users

Model Example

Stirling Engine Adiabatic Model + Losses

Assumptions

-Adiabatic expansion and compression spaces

- Sinusoidal volume variations

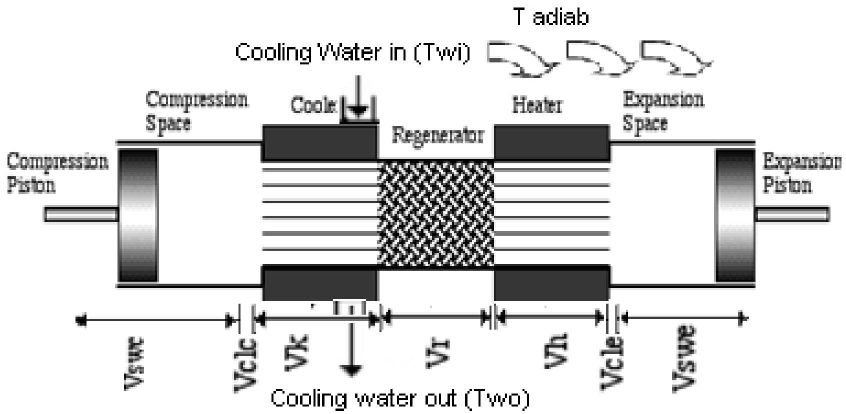
-Ideal gas inside the engine

- Heat Losses

-Friction and Pressure drop losses

-Non ideal Regenerator

- Heat transfer model from the external source to the engine included.



Source: Urielli 2014, http://www.ohio.edu/mechanical/stirling/me422.html

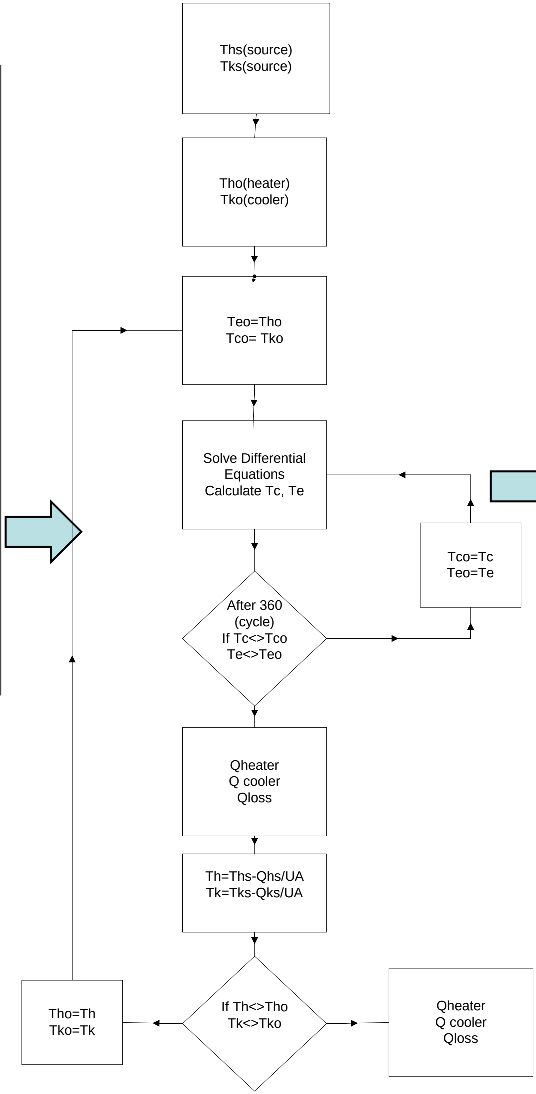
Source: Genoa Stirling, http://www.genoastirling.com/

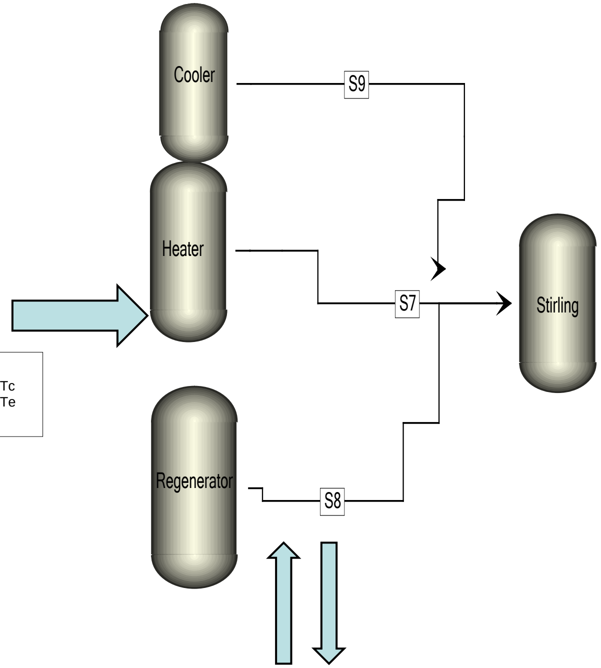
Ideal Adiabatic Losses
Solution Aspen- C++

$p = M R / (V_c / T_c + V_k / T_k + V_r / T_r + V_h / T_h + V_e / T_e)$ $dp = \frac{-\gamma p (dV_c / T_{ck} + dV_e / T_{he})}{[V_c / T_{ck} + \gamma (V_k / T_k + V_r / T_r + V_h / T_h) + V_e / T_{he}]}$	Pressure
$m_c = p V_c / (R T_c)$ $m_k = p V_k / (R T_k)$ $m_r = p V_r / (R T_r)$ $m_h = p V_h / (R T_h)$ $m_e = p V_e / (R T_e)$	Masses
$dm_c = (p\, dV_c + V_c\, dp / \gamma) / (R T_{ck})$ $dm_e = (p\, dV_e + V_e\, dp / \gamma) / (R T_{he})$ $dm_k = m_k\, dp / p$ $dm_r = m_r\, dp / p$ $dm_h = m_h\, dp / p$	Mass Accumulations
$m_{ck}' = -dm_c$ $m_{kr}' = m_{ck}' - dm_k$ $m_{he}' = dm_e$ $m_{rh}' = m_{he}' + dm_h$	Mass Flow
if $m_{ck}' > 0$ **then** $T_{ck} = T_c$ **else** $T_{ck} = T_k$ **if** $m_{he}' > 0$ **then** $T_{he} = T_h$ **else** $T_{he} = T_e$	Conditional Temperatures
$dT_c = T_c (dp / p + dV_c / V_c - dm_c / m_c)$ $dT_e = T_e (dp / p + dV_e / V_e - dm_e / m_e)$	Temperatures
$dQ_k = V_k\, dp\, c_v / R - c_p (T_{ck} m_{ck}' - T_k m_{kr}')$ $dQ_r = V_r\, dp\, c_v / R - c_p (T_k m_{kr}' - T_h m_{rh}')$ $dQ_h = V_h\, dp\, c_v / R - c_p (T_h m_{rh}' - T_{he} m_{he}')$ $dW_c = p\, dV_c$ $dW_e = p\, dV_e$ $dW = dW_c + dW_e$ $W = W_c + W_e$	Energy

+

Pressure Losses	$dQ = \frac{\Delta P m}{\rho}$ $\Delta P = \frac{-2\, fr\, \mu\, \dot{m}\, V}{A d^2 \rho}$
Internal Conducction Heat Exchangers	$dQ = \frac{kA}{L} \Delta T$
Regenerator Losses	$dQ = 1 - \varepsilon (dQri)$
Shuttle Effect Losses	$dQ = \frac{0.4 z^2 kpDd(Td - Tc)}{JLd}$





Solution-complete.c
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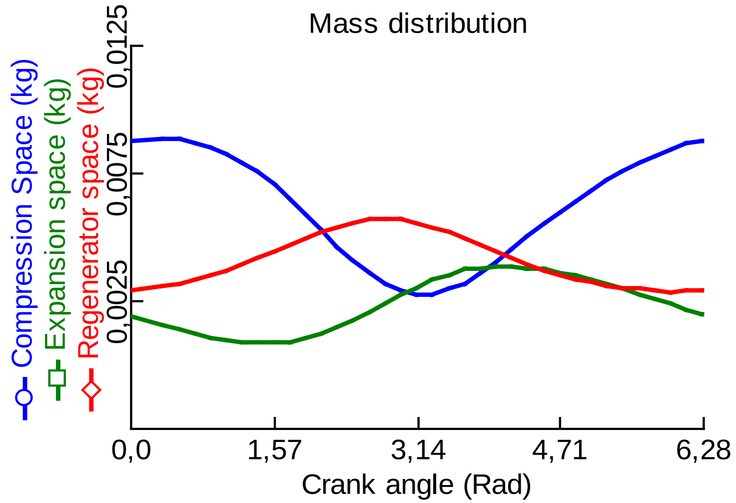
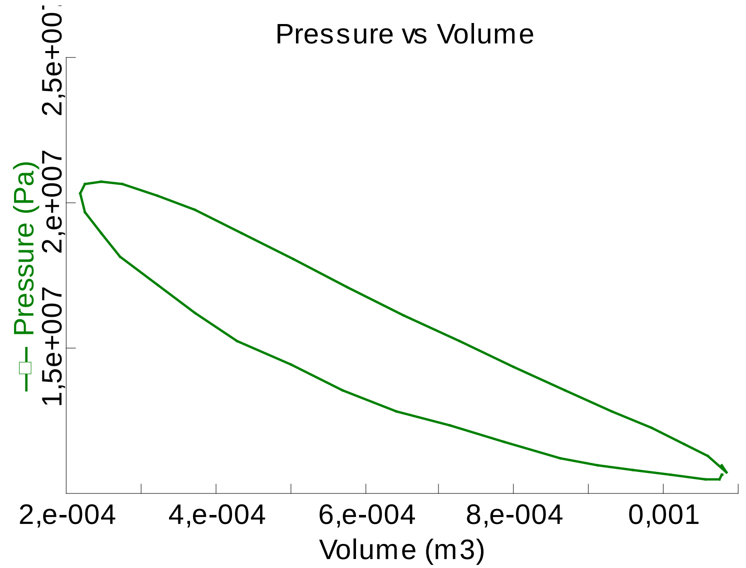
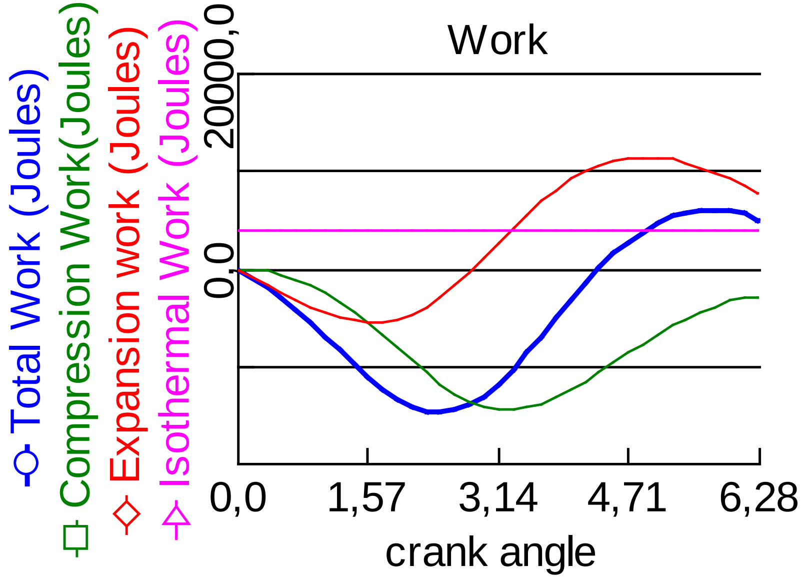
13 KB

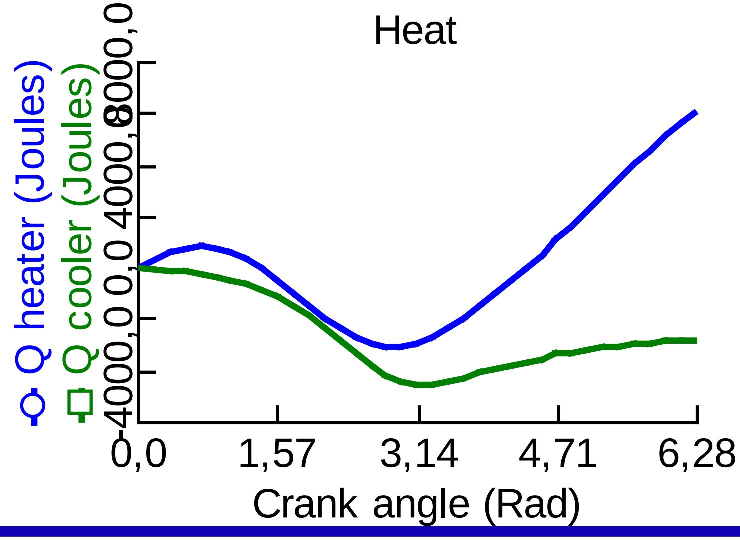
Preliminary Results – Adiabatic model

KTH VETENSKAP OCH KONST









THANKS