



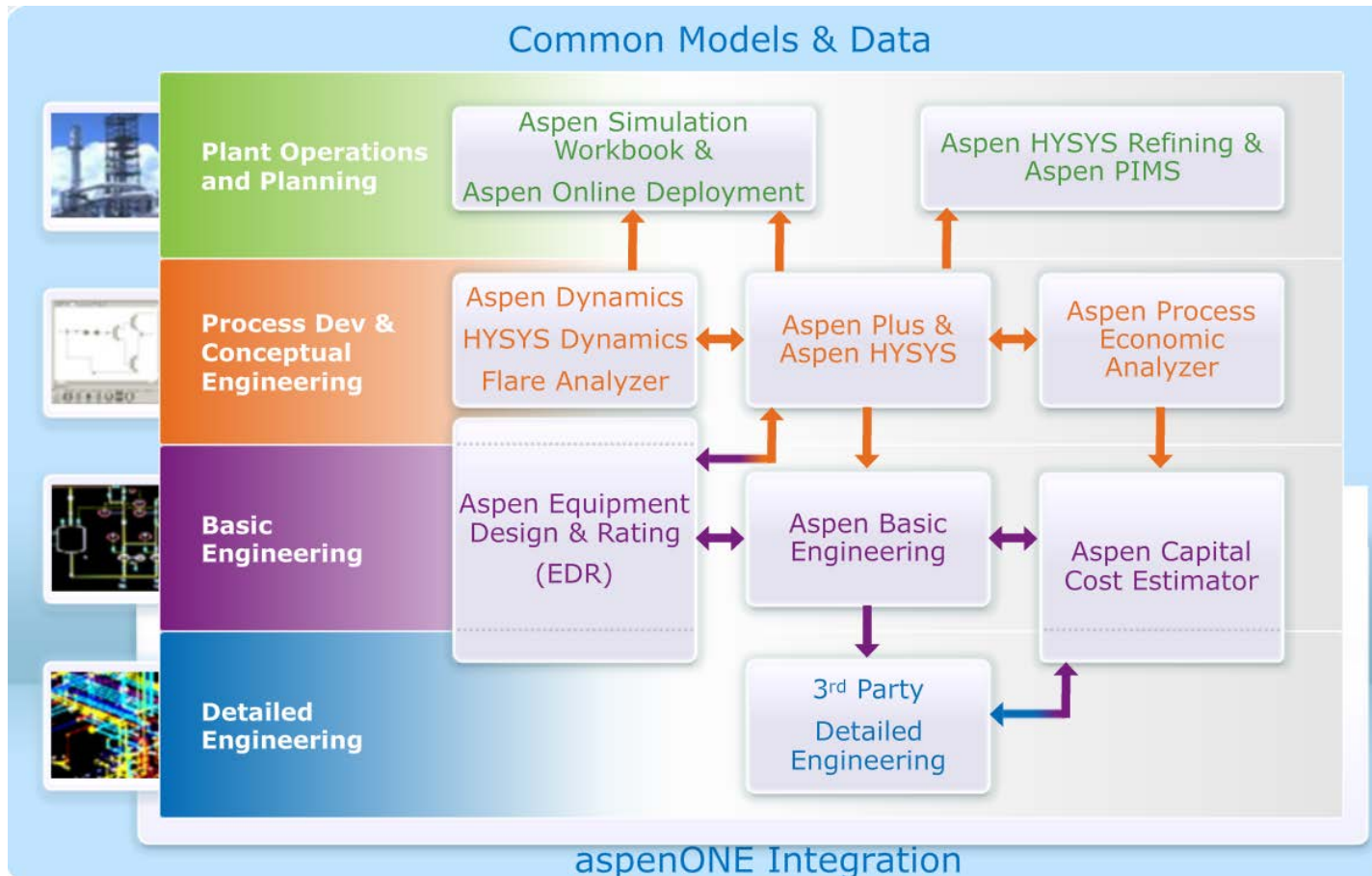
ASPEN ENGINEERING SUITE OVERVIEW



Heat and Power Technology, Stockholm, Sweden

General Overview

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



Source: Aspen Technology, 2012



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ASPEN PLUS

OVERVIEW



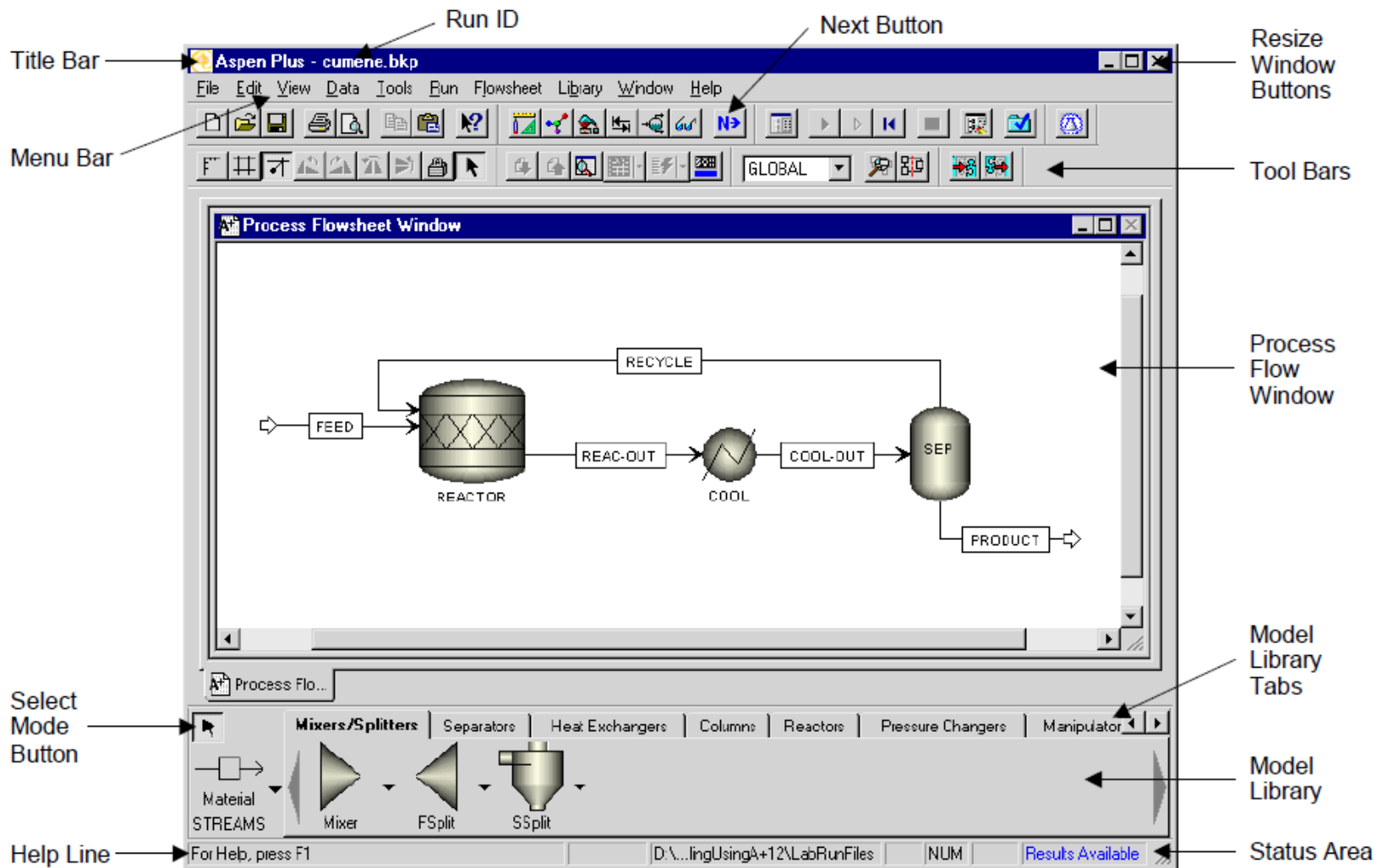
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Aspen Plus

- 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



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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





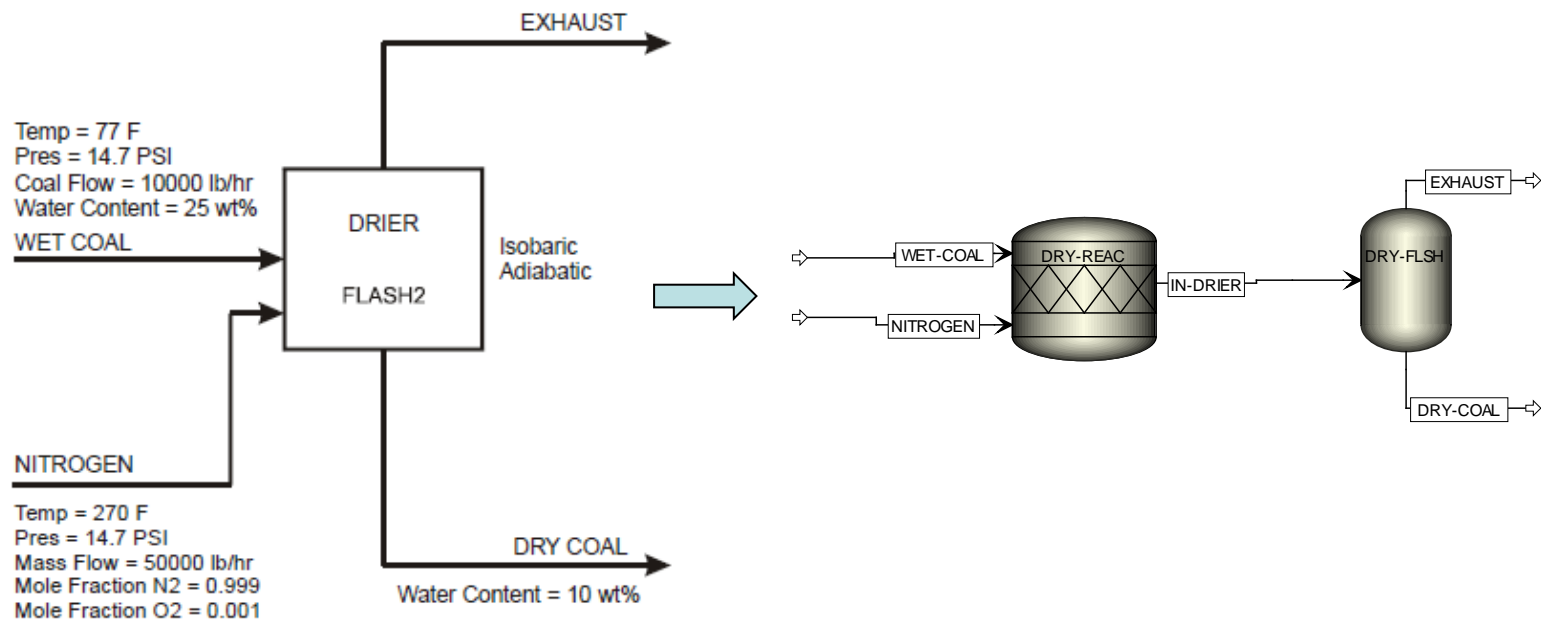
Example



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Define Process Flow Sheet

Coal Drying Flowsheet



Source: Aspen Technology, 2012



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Specify Chemical Components



The screenshot shows the 'Components - Data Browser' window in Aspen Plus V7.2. The window title is 'Simulation 1 - Aspen Plus V7.2 - aspenONE'. The menu bar includes File, Edit, View, Data, Tools, Run, Plot, Library, Costing, Window, and Help. The toolbar contains various icons for file operations and simulation control. The main area is divided into a left-hand tree view and a right-hand data table.

The left-hand tree view shows a hierarchy of simulation components. The 'Components' folder is expanded, showing sub-folders like 'Setup', 'Substreams', 'Costing Op', 'Stream Pricing', 'Units-Sets', 'Custom Un', 'Report Opti', 'Assay/Blendi', 'Light-End F', 'Petro Chara', 'Pseudocom', 'Attr-Comp', 'Henry Com', 'Moisture C', 'UNIFAC Gr', 'Comp-Grou', 'Comp-Lists', 'Polymers', 'Attr-Scaling', 'Properties', 'Flowsheet', 'Streams', 'Blocks', 'Utilities', and 'Reactions'. The 'Components' folder is selected, and the 'Define components' table is visible.

The 'Define components' table has the following columns: Component ID, Type, Component name, and Formula. The table contains the following data:

| Component ID | Type | Component name | Formula |
|--------------|---------------|----------------|---------|
| H2O | Conventional | WATER | H2O |
| N2 | Conventional | NITROGEN | N2 |
| O2 | Conventional | OXYGEN | O2 |
| COAL | Nonconvention | | |
| * | | | |

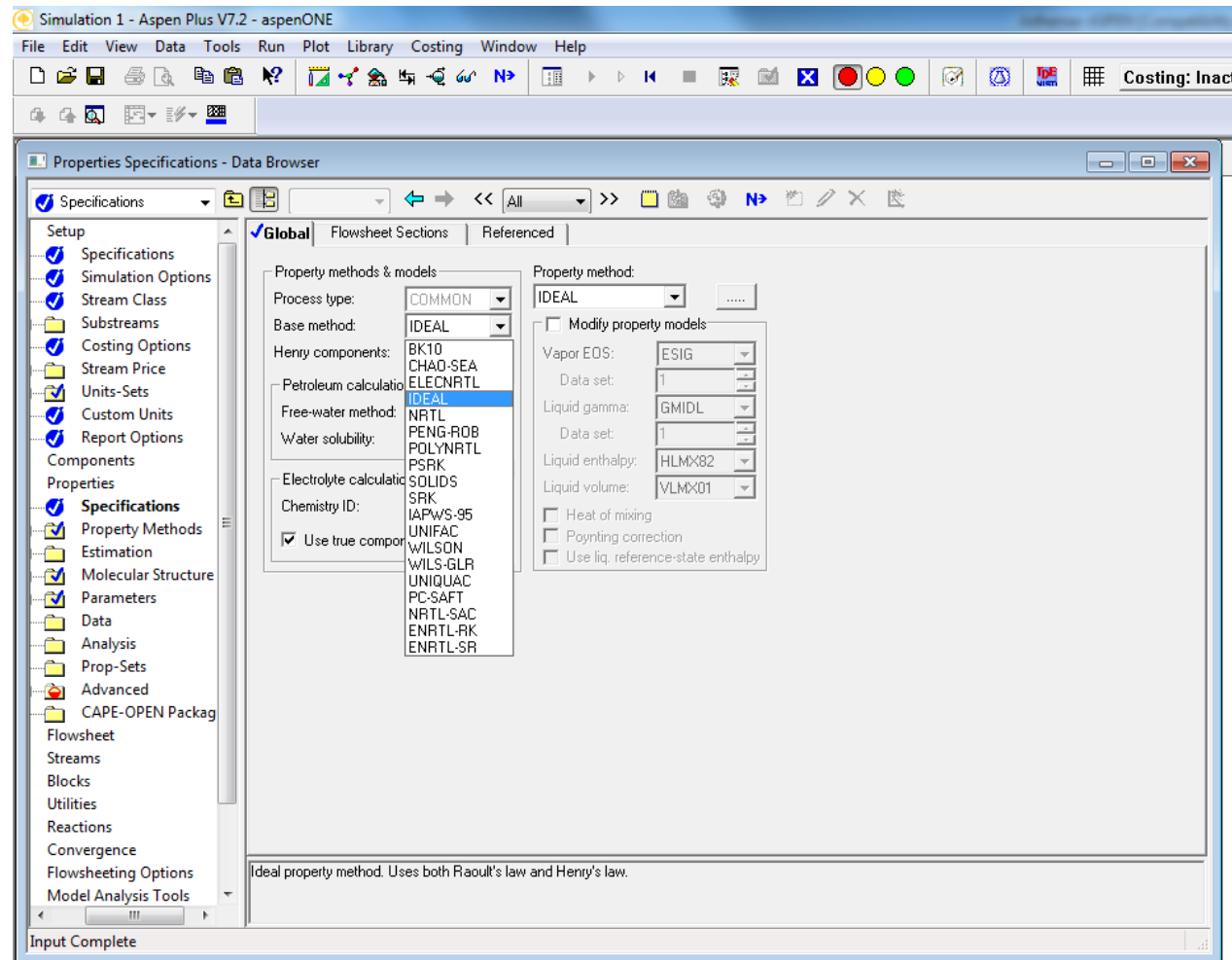
At the bottom of the table, there are buttons for 'Find', 'Elec Wizard', 'User Defined', 'Reorder', and 'Review'. The status bar at the bottom of the window indicates 'Input Complete'.

Source: Aspen Technology, 2012



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Specify Thermodynamic Model



Source: Aspen Technology, 2012



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Specify Flow Rates conditions



The screenshot shows the 'Stream NITROGEN (MATERIAL) Input - Data Browser' window in Aspen Plus. The 'Specifications' tab is active, showing the following settings:

- Substream name: **MIXED**
- State variables:
 - Temperature: 270 F
 - Pressure: 14.7 psia
- Total flow: 50000 lbmol/hr
- Composition (Mass-Frac):

| Component | Value |
|-----------|-------|
| H2O | |
| N2 | 0.999 |
| O2 | 0.001 |
- Total: 1

Source: Aspen Technology, 2012



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Simulation Results



Results Summary Custom Stream Summary - Data Browser

Custom Stream Summ

| | | 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 | | | | | | |
| Default / | | | | | | |

Input Changed

Source: Aspen Technology, 2012



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ASPEN CUSTOM MODELER



OVERVIEW



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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 others



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.

Graphical User Interface

The screenshot shows the Aspen Custom Modeler 2004 interface. Annotations with red arrows point to various components: 'Menus' points to the top menu bar; 'Help' points to the Help menu; 'Run mode' points to the 'Dynamic' dropdown; 'Run button' points to the play button; 'Explorer' points to the left-hand tree view; 'Contents of selected object' points to the 'Contents of Flowsheet' table; 'Flowsheet' points to the central process diagram; 'simulation messages' points to the bottom status bar; and 'Specification status' points to the 'Ready' indicator.

| Name | Type |
|----------------|---------------|
| Flowsheet | Folder |
| LocalVariables | Table |
| Streams | Folder |
| Tasks | Task |
| Plots/Plots... | Plot/Plots... |

| Component | Value | Spec | Units |
|----------------|---------|------|--------------------|
| Component: out | Default | | |
| p_in Component | Default | | |
| p_in F | 160 | Free | m ³ /hr |
| Flow Control | Default | | |

Simulation Messages:
Step 166: Time = 6.15, step = 0.05 accepted.
Integrating from 6.15 to 6.2
Step 167: Time = 6.2, step = 0.05 accepted, error/tol = 0
Run paused at 11:18

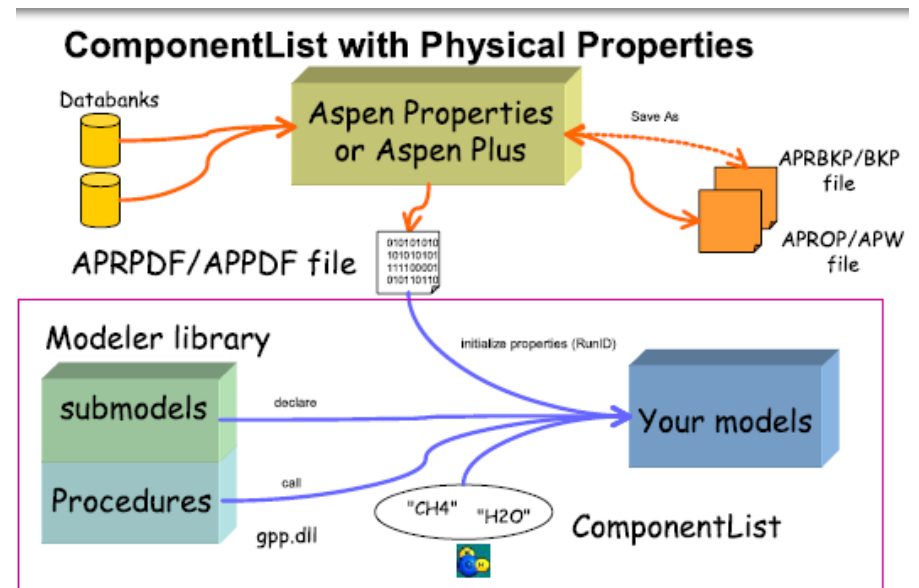
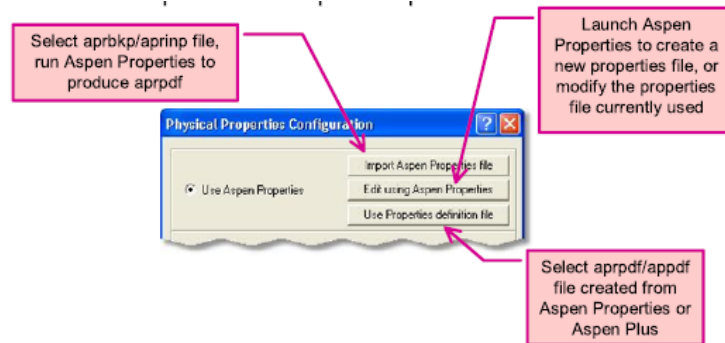
Source: Aspen Technology, 2012



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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



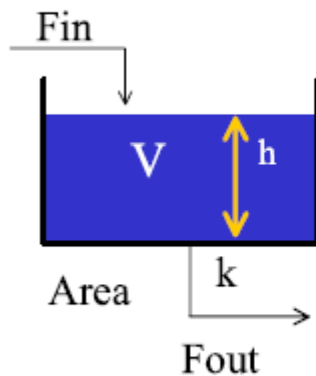
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Features

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

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

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

$$V = A \cdot h$$

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;
    
```

| | Value | Spec | Units |
|---------------|---------|-------|--------------------|
| A | 1.0 | Fixed | m ² |
| ComponentList | Default | | |
| Fi | 1.0 | Fixed | m ³ /hr |
| Fo | 1.0 | Free | m ³ /hr |
| h | 1.0 | Free | m |
| k | 1.0 | Fixed | |
| V | 10.0 | Free | m ³ |

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

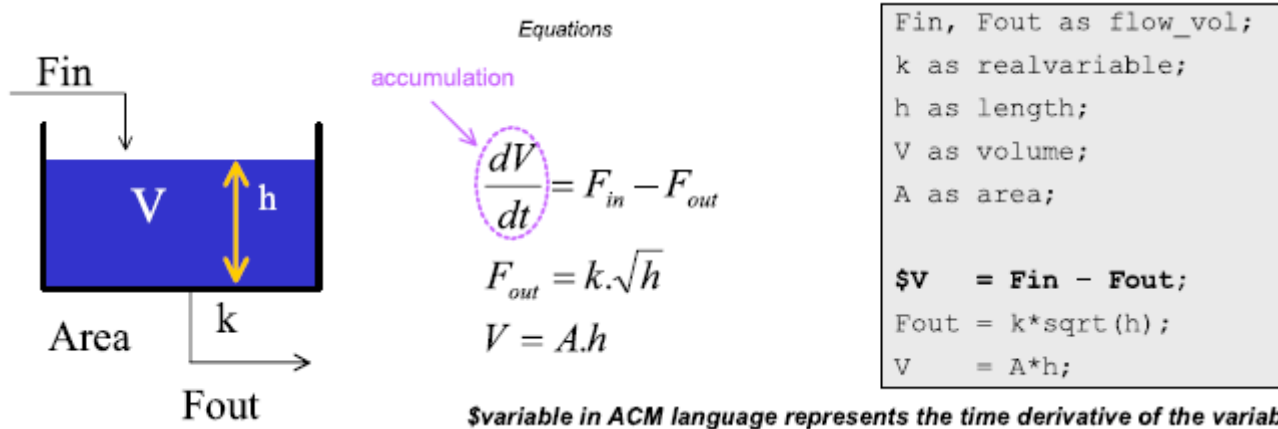
Source: Aspen Technology, 2012



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Features

- System of **differential and algebraic equations**



```

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



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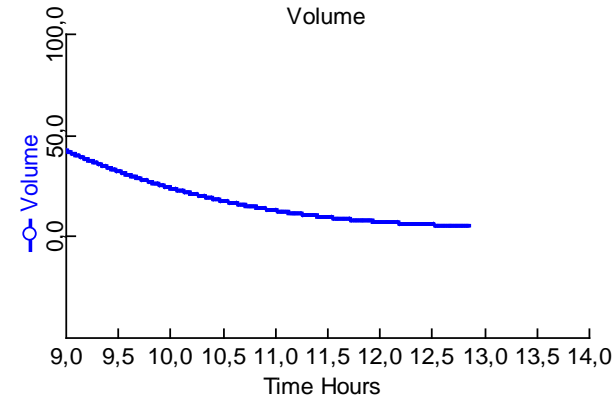
Features

Flexible user-defined forms

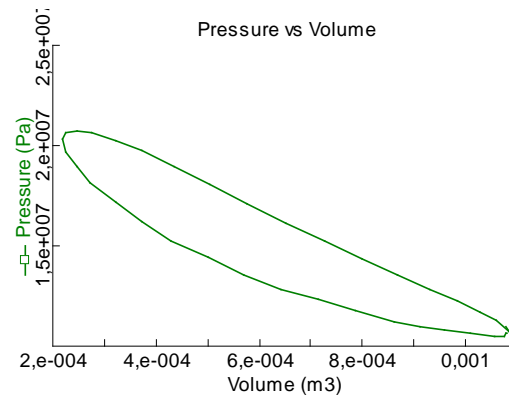


| Time | B1.v | B1.h | B1.Fout |
|-------|---------|---------|---------|
| Hours | m3 | m | m3/hr |
| 0,0 | 100,0 | 100,0 | 50,0 |
| 0,01 | 99,6008 | 99,6008 | 49,9002 |
| 0,02 | 99,2028 | 99,2028 | 49,8004 |
| 0,03 | 98,8057 | 98,8057 | 49,7006 |
| 0,04 | 98,4102 | 98,4102 | 49,6008 |
| 0,05 | 98,0146 | 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 |

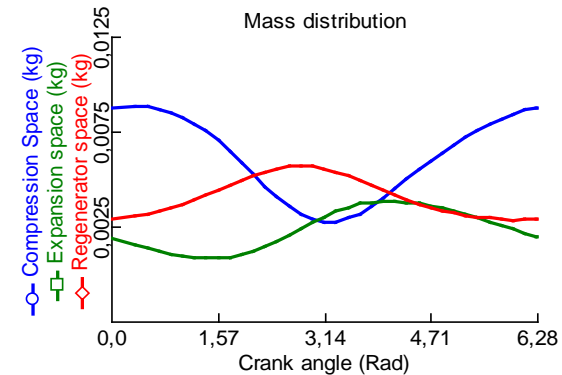
Table Forms



Time series Plot forms



Phase Plots



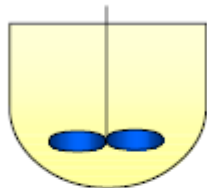
Profile Plots



Features

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

Estimation example

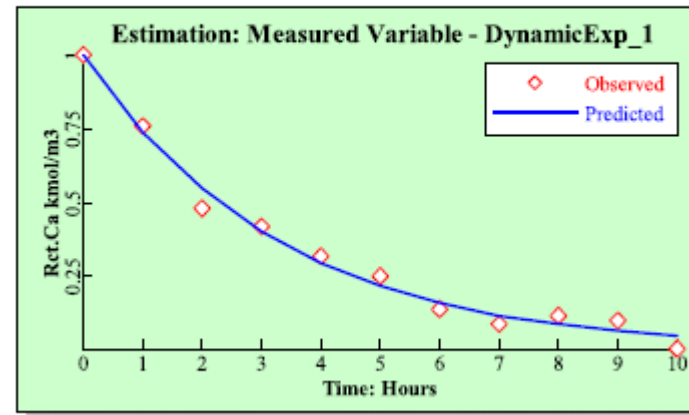


$$r = k_0 \cdot e^{-E/RT} \cdot C_A^a$$

$$dC_A/dt = -r$$

$$dC_B/dt = r$$

$k_0 = 9.74$ (standard deviation 0.39)



Source: Aspen Technology, 2012

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



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Features

Optimization example

Dynamic Optimization

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

subject to

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

$$0 \leq t \leq t_f$$

$$\left. \begin{aligned} C(\dot{x}(t_f), x(t_f), z(t_f)) &= 0 \\ C(\dot{x}(t_f), x(t_f), z(t_f)) &\geq 0 \end{aligned} \right\} \text{Constraints}$$

$$L(i) \leq \{u_i(t), v(i)\} \leq U(i) \quad \text{Decision and control variables}$$

Objective

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

Constraints

Maximum reactor temperature over time;
Final concentration of components

Decision and control variables

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



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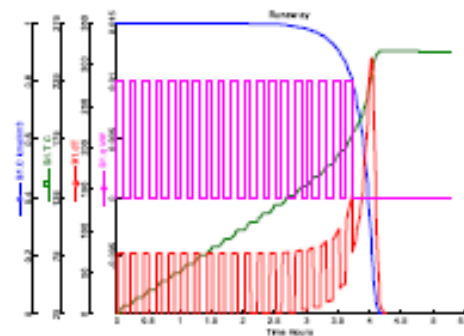
Features

- **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

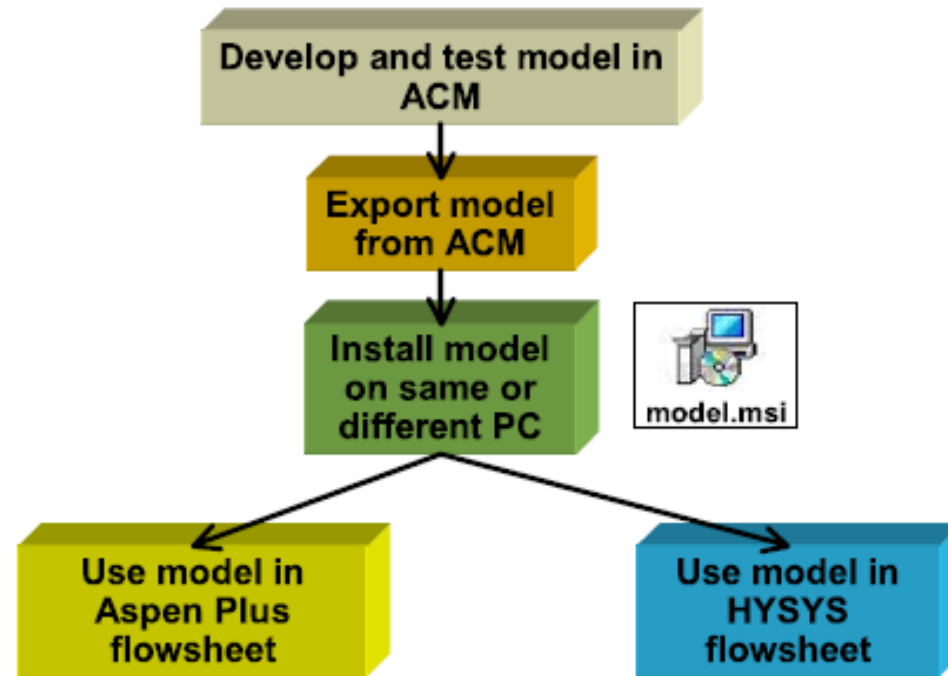


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Features

- Export Equipments or process models

Workflow



Source: Aspen Technology, 2012



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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

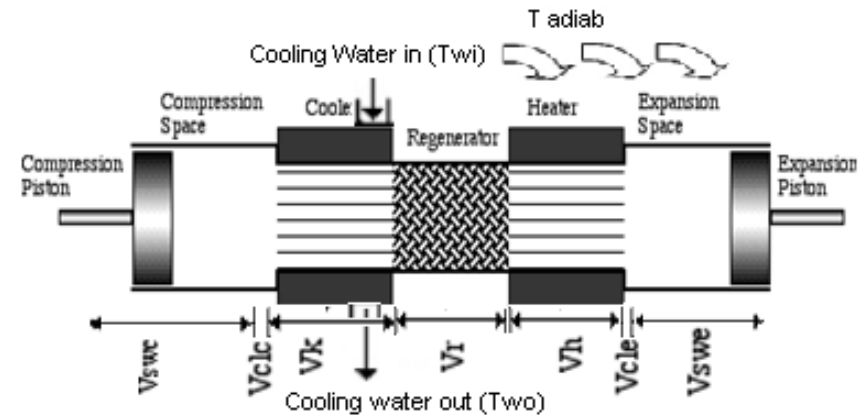


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Stirling Engine Adiabatic Model + Losses

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/>



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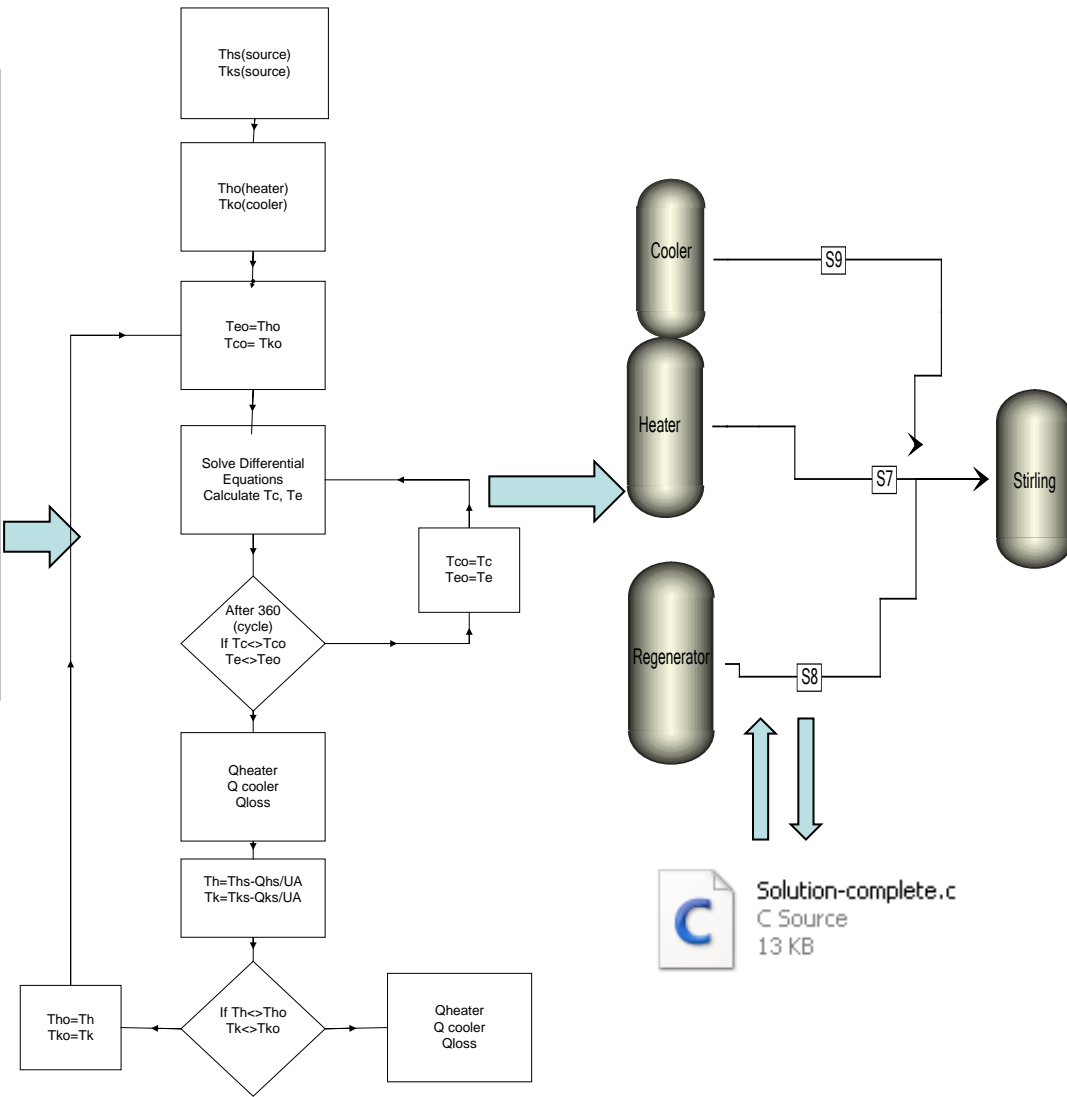
Department of Energy Technology

Ideal Adiabatic Losses Solution Aspen- C++

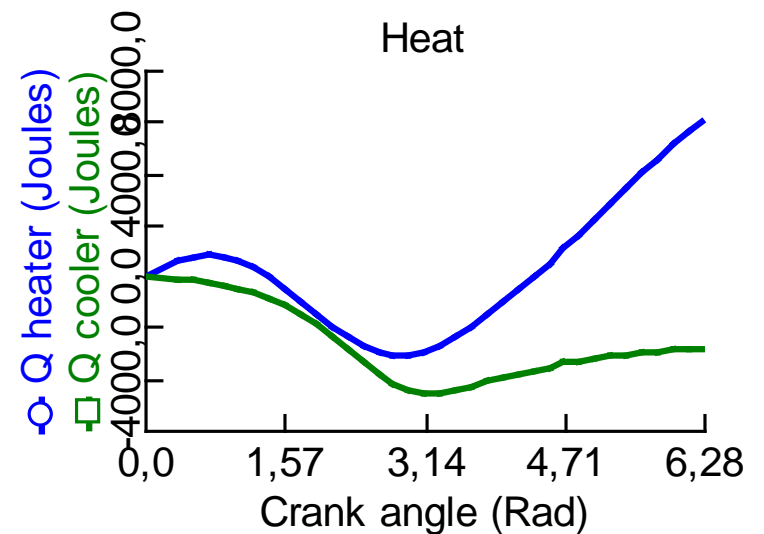
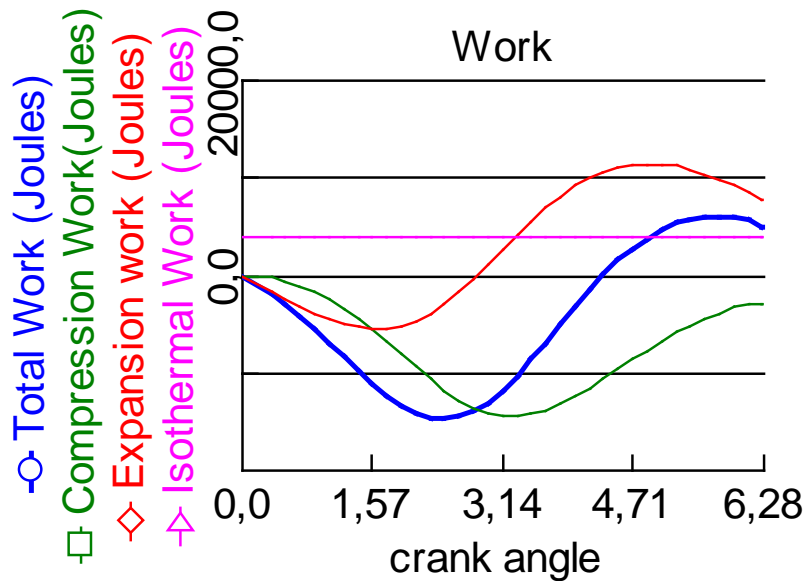
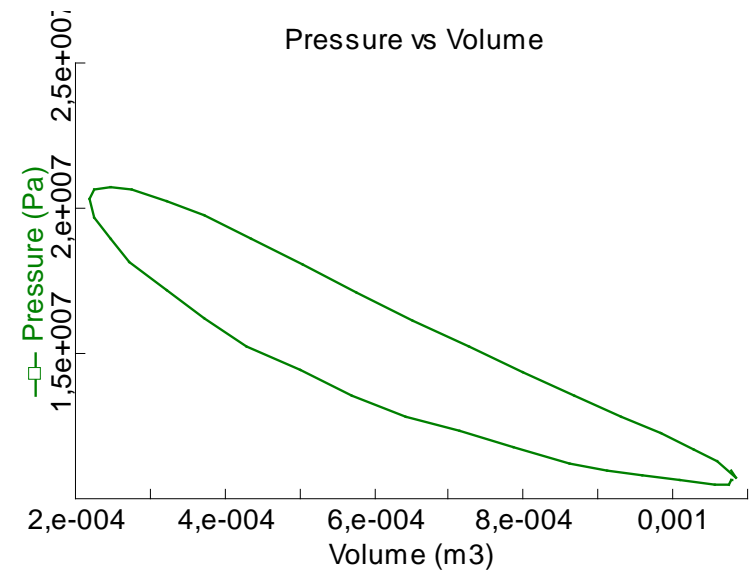
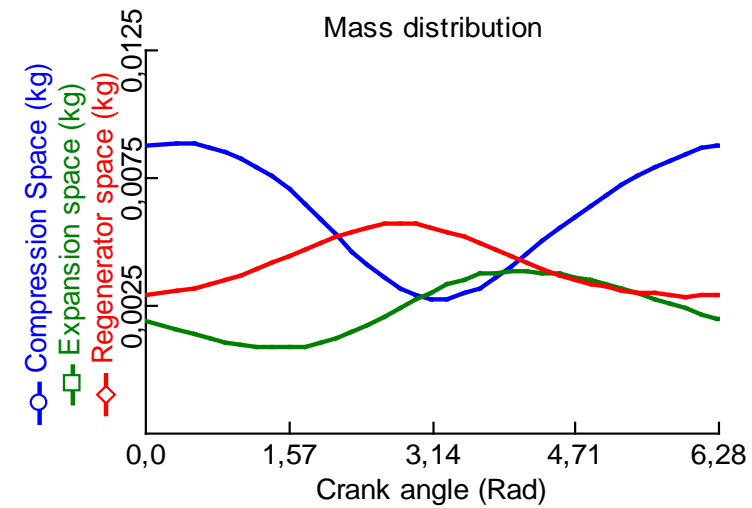


| | |
|--|--------------------------|
| $p = M R / (V_c / T_c + V_k / T_k + V_r / T_r + V_h / T_h + V_e / T_e)$ $dp = \frac{-\gamma p (dV_c / T_c k + dV_e / T_e h)}{[V_c / T_c k + \gamma (V_k / T_k + V_r / T_r + V_h / T_h) + V_e / T_e h]}$ | Pressure |
| $m_c = p V_c / (R T_c)$ $m_k = p V_k / (R T_k)$ $m_r = p V_r / (R T_r)$ $m_h = p V_h / (R T_h)$ $m_e = p V_e / (R T_e)$ | Masses |
| $dm_c = (p dV_c + V_c dp / \gamma) / (R T_c k)$ $dm_e = (p dV_e + V_e dp / \gamma) / (R T_e h)$ $dm_k = m_k dp / p$ $dm_r = m_r dp / p$ $dm_h = m_h dp / p$ | Mass Accumulations |
| $mck' = -dm_c$ $mkr' = mck' - dm_k$ $mhr' = dm_e$ $mre' = mhr' + dm_r$ | Mass Flow |
| if $mck' > 0$ then $Tck = Tc$ else $Tck = Tk$ if $mhr' > 0$ then $The = Th$ else $The = Te$ | 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 |
| $dQ_k = V_k dp cv / R - cp (Tck mck' - Tk mkr')$ $dQ_r = V_r dp cv / R - cp (Tk mkr' - Th mhr')$ $dQ_h = V_h dp cv / R - cp (Th mhr' - The mhe')$ $dW_c = p dV_c$ $dW_e = p dV_e$ $dW = dW_c + dW_e$ $W = W_c + W_e$ | Energy |

| | |
|-------------------------------------|---|
| Pressure Losses | $dQ = \frac{\Delta P m}{\rho}$ $\Delta P = \frac{-2 f r \mu m V}{A d^2 \rho}$ |
| Internal Conduction Heat Exchangers | $dQ = \frac{kA}{L} \Delta T$ |
| Regenerator Losses | $dQ = 1 - \epsilon (dQ_{ri})$ |
| Shuttle Effect Losses | $dQ = \frac{0.4 z^2 k p D d (T_d - T_c)}{J L d}$ |



Preliminary Results – Adiabatic model



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THANKS



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