NATIONAL ENERGY TECHNOLOGY LABORATORY

2012 AIChE Meeting, Pittsburgh, PA

Enforcing Elemental Mass and Energy Balances for Reduced Order Models

Jinliang Ma [1, 4], Christopher Montgomery [1, 4], Khushbu Agarwal [2], Poorva Sharma [2], Yidong Lang [5], David Huckaby[1] , Stephen Zitney [1], Ian Gorton [2], Deb Agawal [3], David Miller [1]

[1]U.S. DOE/National Energy Technology Laboratory, Morgantown, WV 26507

[2]U.S. DOE/Pacific Northwest National Laboratory, Richland, WA 99352

[3]U.S. DOE/Lawrence Berkeley National Laboratory, Berkeley, CA 94720

[4]URS Corporation, Morgantown, WV 26505

[5]Carnegie Mellon University, Pittsburgh, PA 15213

This technical effort was performed in support of DOE's Carbon Capture Simulation Initiative (CCSI) project under the RES contract RES0004000.2.600.232.001

Introduction

Multi-Scale Models in Carbon Capture Simulation Initiative (CCSI)

https:www.acceleratecarboncapture.org

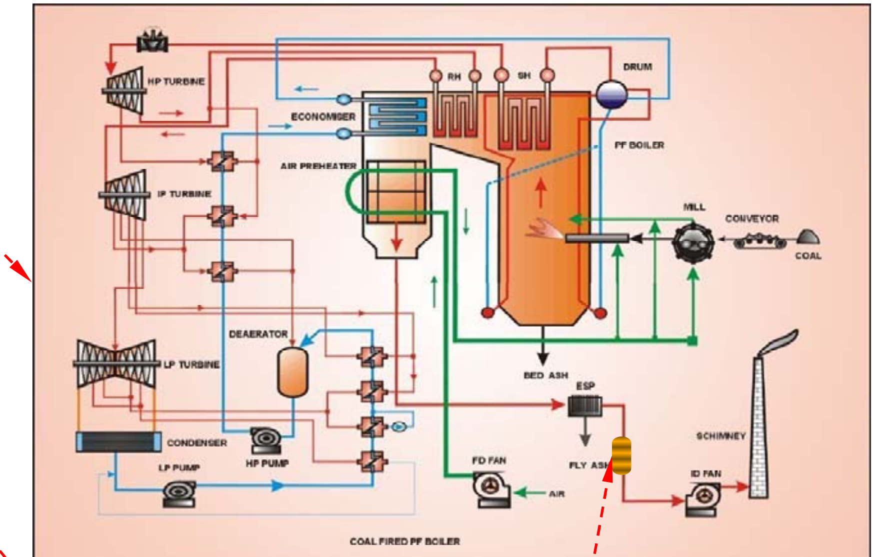
Scale

Plant Scale
- Process (Aspen Plus, gPROMS)

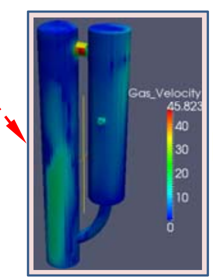
Device Scale
- 1-D Reactor
- Computational Fluid Dynamics

Single Particle Scale
- Diffusion (Film, Pore)
- Surface Adsorption/Reactions

Molecule Scale
- Molecular Dynamics
- Computational Chemistry



Power Plant Process Model

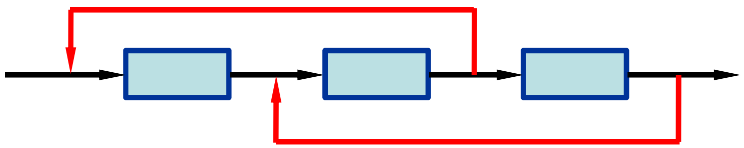


ROM

CO_2 Adsorber Model (CFD)

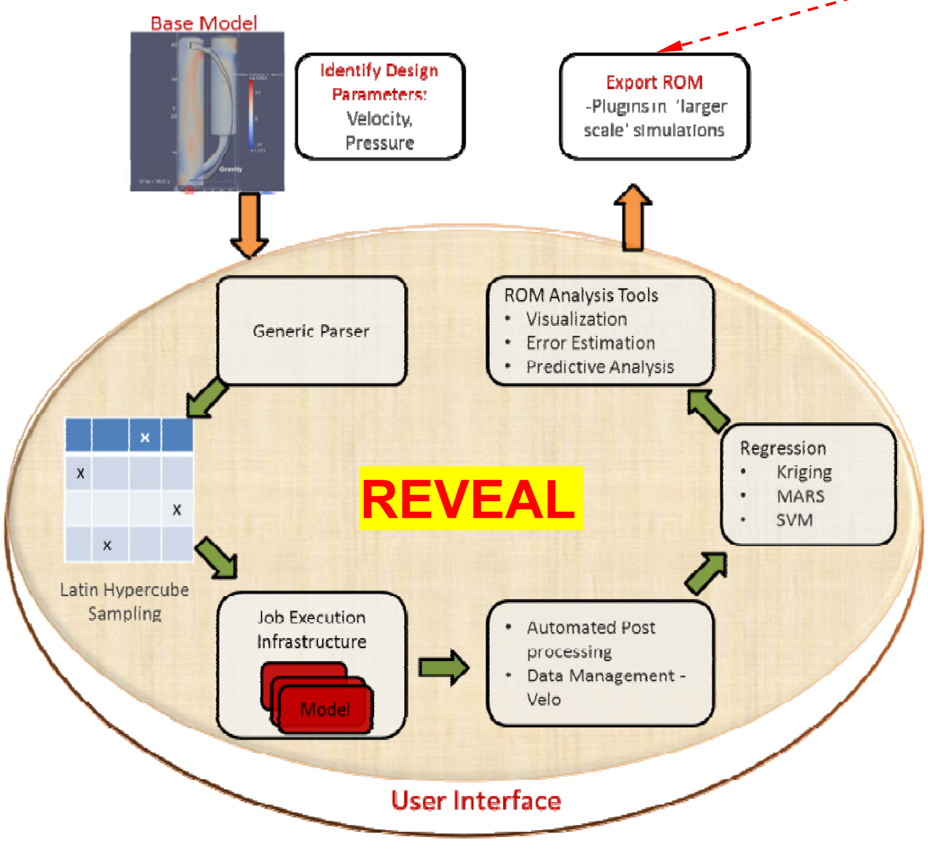
High-Fidelity Model Versus ROM

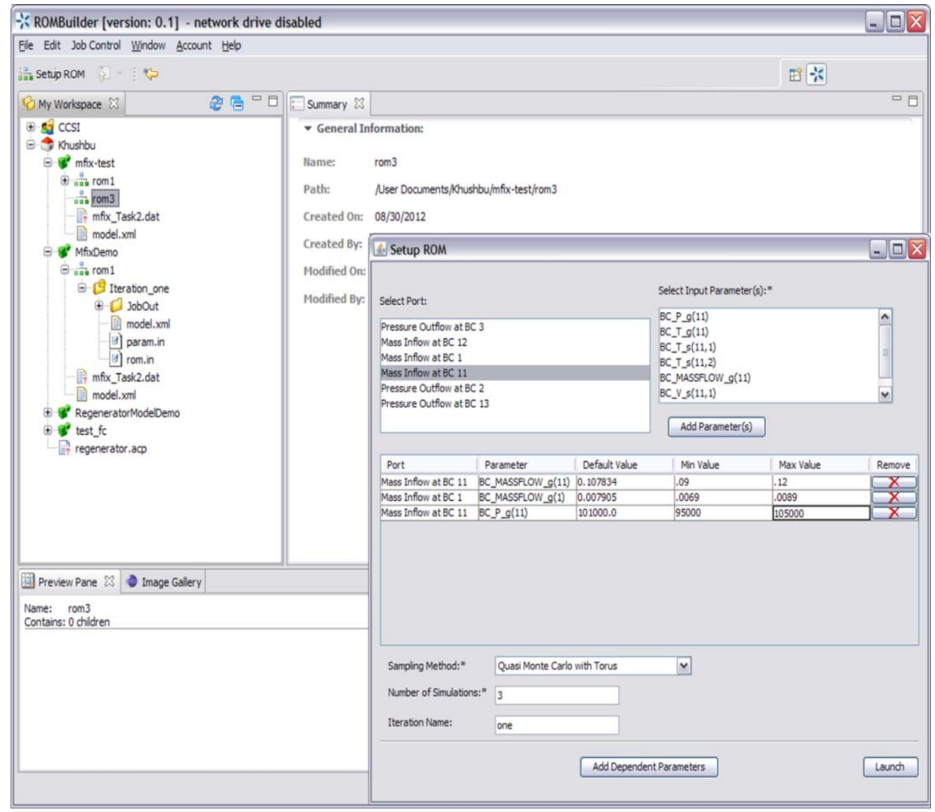
- **High-Fidelity Model**
  - e.g. CFD, Ideal Reactors (Equilibrium, Plug Flow, CSTR)
  - Based on first principles
  - Usually conserves mass/energy
    - If converged tightly
  - Slow (CPU Intensive)
- **Reduced Order Model (ROM)**
  - Based on mathematical regression/interpolation
    - Kriging
    - Artificial Neural Network (ANN)
    - Others
  - Not necessarily conserves mass/energy
  - Possible unrealistic predictions (negative species mass flow rates)
  - Fast
- **ROM as a Bridge Between Multiple Scales**
  - Needs tight mass/energy balances
    - Important for recycles



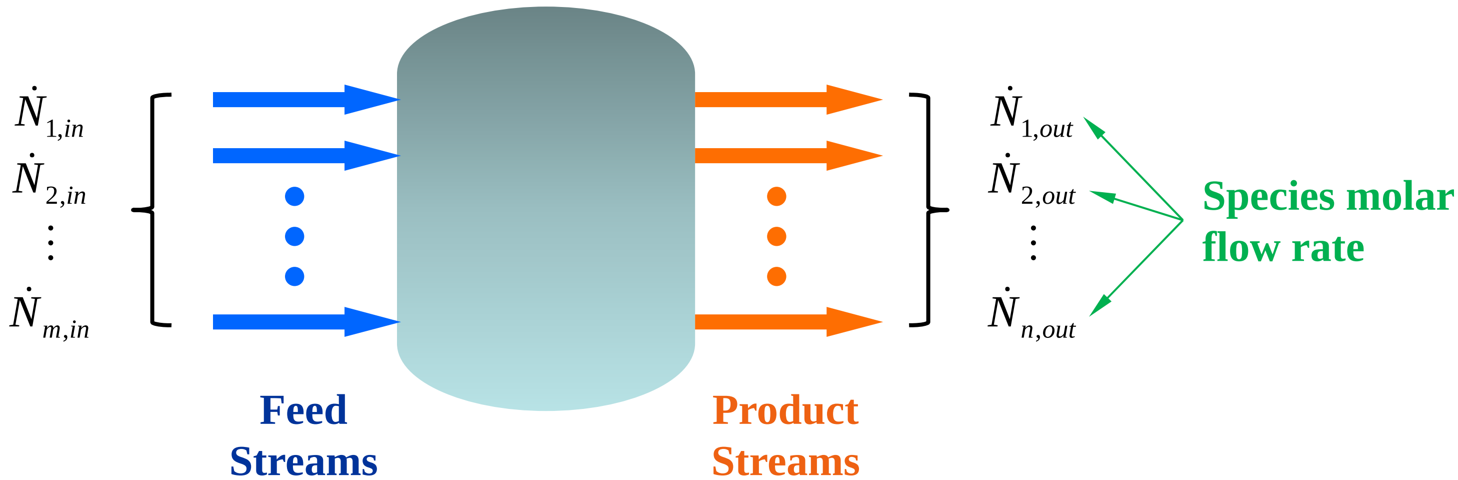
REVEAL: CCSI’s ROM Generation Software

In a form of unit operation model for PME (e.g. Aspen Plus, ACM, gPROMS)





Enforcing Mass Balance



For each mole of species *i*, there are $A_{i,j}$ moles of element *j* (*j*=1,2,…,*l*)
e.g., for CH_4, $A_{1,1}$=4, $A_{1,2}$=1, $A_{1,3}$=0, $A_{1,4}$=0

For element *j*: $\dot{L}_{j,in} = \sum_{i=1}^{m} \dot{N}_{i,in} A_{i,j}$ $\qquad \dot{L}_{j,out} = \sum_{i=1}^{n} \dot{N}_{i,out} A_{i,j}$

Mass balance: $\sum_{i=1}^{m} \dot{N}_{i,in} A_{i,j} = \sum_{i=1}^{n} \dot{N}_{i,out} A_{i,j}$ $\qquad$ (*j*=1,2,…,*l*)

Correction Factors For Product Species

For product species *i*, Define:

$$f_i \equiv \frac{\dot{N}_{i,out} - \dot{N}_{i,out}^{ROM}}{\dot{N}_{i,out}^{ROM}} = \frac{\dot{N}_{i,out}}{\dot{N}_{i,out}^{ROM}} - 1$$

Corrected Prediction ($\dot{N}_{i,out}$)

ROM Prediction ($\dot{N}_{i,out}^{ROM}$)

Corrected molar flow of species *i*: $\dot{N}_{i,out} = (1 + f_i)\dot{N}_{i,out}^{ROM}$

Eqn. for solving f_i:

$$\sum_{i=1}^{m} \dot{N}_{i,in} A_{i,j} = \sum_{i=1}^{n} (1 + f_i)\dot{N}_{i,out}^{ROM} A_{i,j}$$

Let $\Delta \dot{L}_j \equiv \sum_{i=1}^{m} \dot{N}_{i,in} A_{i,j} - \sum_{i=1}^{n} \dot{N}_{i,out}^{ROM} A_{i,j}$ **(Mass imbalance)**

Then $\sum_{i=1}^{n} f_i \dot{N}_{i,out}^{ROM} A_{i,j} - \Delta \dot{L}_j = 0$ **(Based on element *j*)**

Number of equations: *l* (one for each element)

Number of unknowns: *n* (one for each product species)

Notes: 1.Total mass will be balanced if individual elements are balanced.

2. if $\dot{N}_{i,out}^{ROM} < 0$, set it to a small positive number. Use $-0.01\dot{N}_{i,out}^{ROM}$

Solving Correction Factors

Scenario 1: $n>l$

Approach: Find most reasonable correction factors by **minimizing** $\sum_{i=1}^{n} f_i^{\,2}$ while enforcing mass balance for each element

Algorithm: **Lagrangian multiplier method** (mass balance equations as constraints)

Lagrangian Function G:

$$G(f_1, f_2, \cdots, f_n, \lambda_1, \lambda_2, \cdots, \lambda_l) = \sum_{i=1}^{n} f_i^{\,2} + \sum_{j=1}^{l} \lambda_j \left(\sum_{i=1}^{n} f_i \dot{N}_{i,out}^{ROM} A_{i,j} - \Delta \dot{L}_j \right)$$

Partial Derivatives of G:

$$\frac{\partial G}{\partial f_i} = 2 f_i + \dot{N}_{i,out}^{ROM} \sum_{j=1}^{l} A_{i,j} \lambda_j = 0 \qquad (i = 1,2,\cdots,n)$$

$$\frac{\partial G}{\partial \lambda_j} = \sum_{i=1}^{n} \dot{N}_{i,out}^{ROM} A_{i,j} f_i - \Delta L_j = 0 \qquad (j = 1,2,\cdots,l)$$

Total number of equations: $n+l$

Total number of unknowns: $n+l$

Solving Correction Factors

Scenario 2: $n<l$

Example: CO_2 and H_2O as products (2 species, 3 elements)

Approach: Find best fit for correction factors by least square solution

$$\sum_{i=1}^{n} \dot{N}_{i,out}^{ROM} A_{i,j} f_i = \Delta \dot{L}_j \left(j = 1,2,\cdots,l \right) \rightarrow M\vec{f} = \vec{b}$$

(Matrix M is $l \times n$)

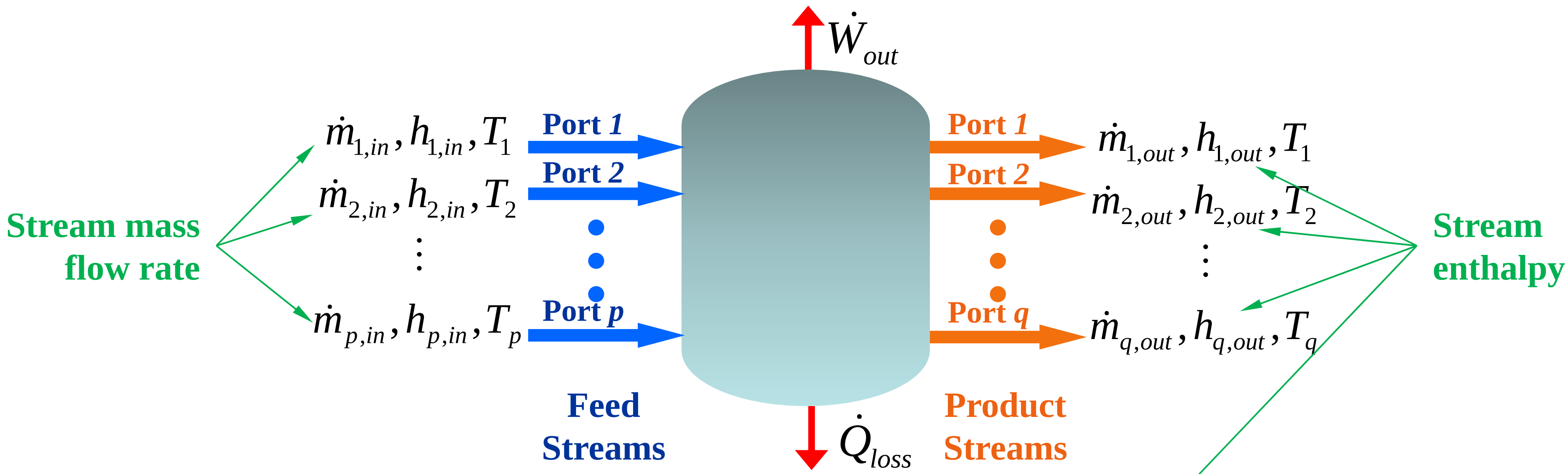
Algorithm: Minimize quadratic $\left\| M\vec{f} - \vec{b} \right\|^2$ (Linear Least Square Method)

Solve: $\left(M^T M \right) \vec{f} = M^T \vec{b}$ (Product matrix $\left(M^T M \right)$ is $n \times n$)

Total number of equations: n
Total number of unknowns: n

Note: Applicable to non-reacting devices

Enforcing Energy Balance



Stream Enthalpy: $$h_{mix}(T) = \sum_{k=1}^{s} y_k \left[h_{f,k}^{o} + \int_{T_0}^{T} C_{p,k}(T')dT' \right]$$ **(If ideal gas mixture)**

Enthalpy Rate In: $$\dot{H}_{in} = \sum_{i=1}^{p} \dot{m}_{i,in} h_{i,in}$$

Enthalpy Rate Out: $$\dot{H}_{out} = \sum_{i=1}^{q} \dot{m}_{i,out} h_{i,out}$$

Energy Balance: $$\sum_{i=1}^{p} \dot{m}_{i,in} h_{i,in} = \sum_{i=1}^{q} \dot{m}_{i,out} h_{i,out} + \dot{W}_{out} + \dot{Q}_{loss}$$

Enforcing Energy Balance

Option 1: Adjusting heat loss

$$\dot{Q}_{loss} = \sum_{i=1}^{p} \dot{m}_{i,in} h_{i,in} - \sum_{i=1}^{q} \dot{m}_{i,out} h_{i,out}^{ROM} - \dot{W}_{out}^{ROM}$$

Option 2: Adjusting product stream enthalpy/temperature

Total Enthalpy Rate of Products:

$$\dot{H}_{out} = \dot{H}_{in} - \dot{W}_{out}^{ROM} - Q_{loss}^{ROM}$$

Total Enthalpy Rate Correction:

$$\Delta\dot{H}_{out} = \dot{H}_{out} - \dot{H}_{out}^{ROM} = \dot{H}_{in} - \dot{W}_{out}^{ROM} - Q_{loss}^{ROM} - \dot{H}_{out}^{ROM}$$

Enthalpy Rate Correction for Port *i*:

$$\Delta\dot{H}_{i,out} = \frac{\dot{m}_{i,out}}{\sum_{j=1}^{q} \dot{m}_{j,out}} \Delta\dot{H}_{out}$$

Enthalpy Correction Per Unit Mass for Port *i* :

$$\Delta h_{i,out} = \frac{\Delta\dot{H}_{out}}{\sum_{j=1}^{q} \dot{m}_{j,out}}$$

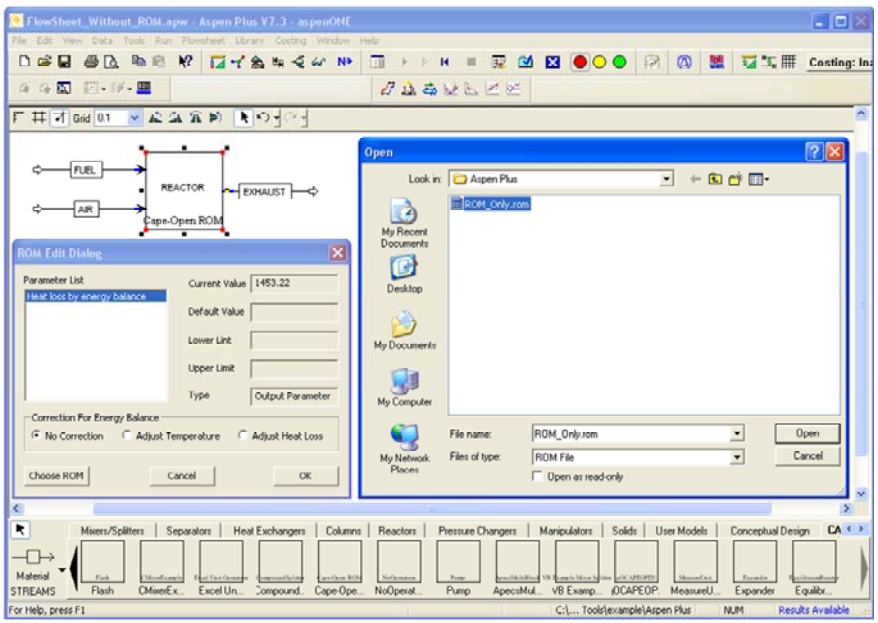
Solve Temperature T_i for Port *i* :

$$\Delta h_{i,out} = \int_{T_i^{ROM}}^{T_i} C_{p,i}(T')dT'$$

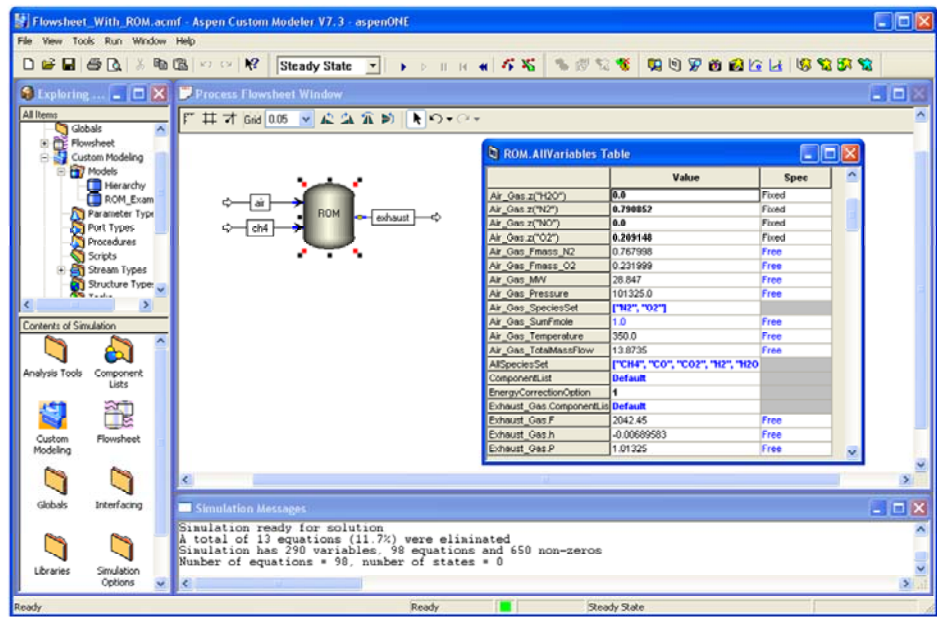
(for product port *i*)

Implementations

- CAPE-OPEN Unit Operation Model
  - Aspen Plus, gPROMS, COFE
- Generation of Vendor Specific Source Code (Custom Model)
  - Aspen Custom Modeler (Equation-Oriented)
  - gPROMS (Equation-Based)



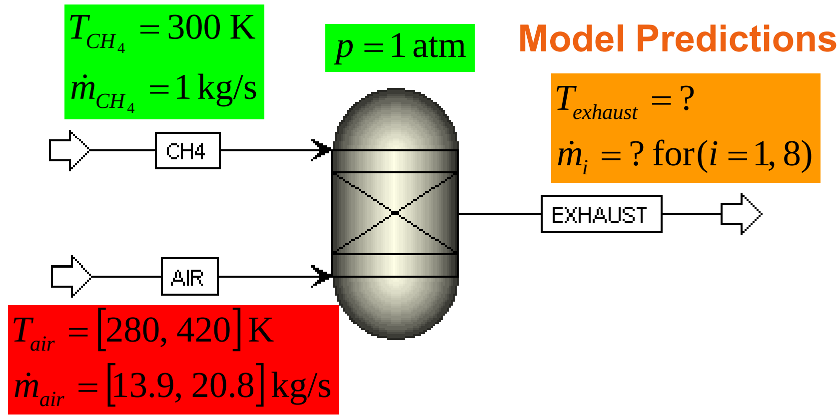
Aspen Plus through CAPE-OPEN

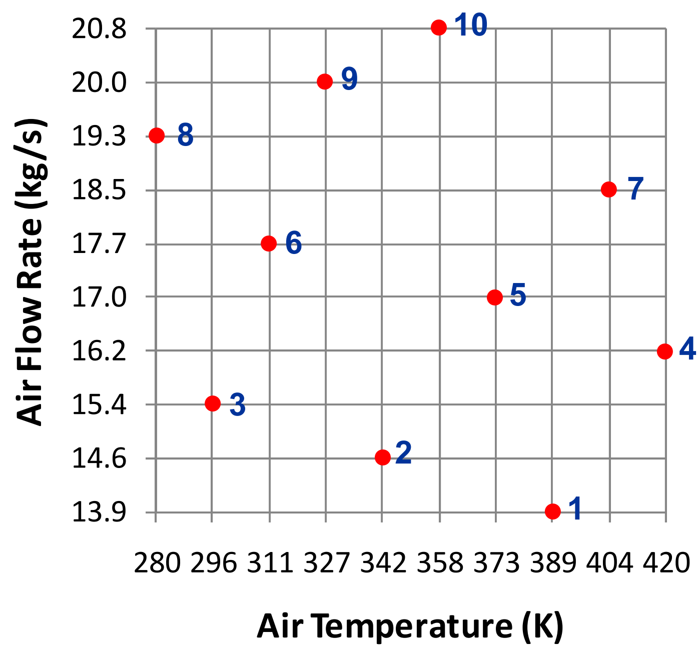


ACM through Custom Model

Example: Equilibrium Flow Reactor

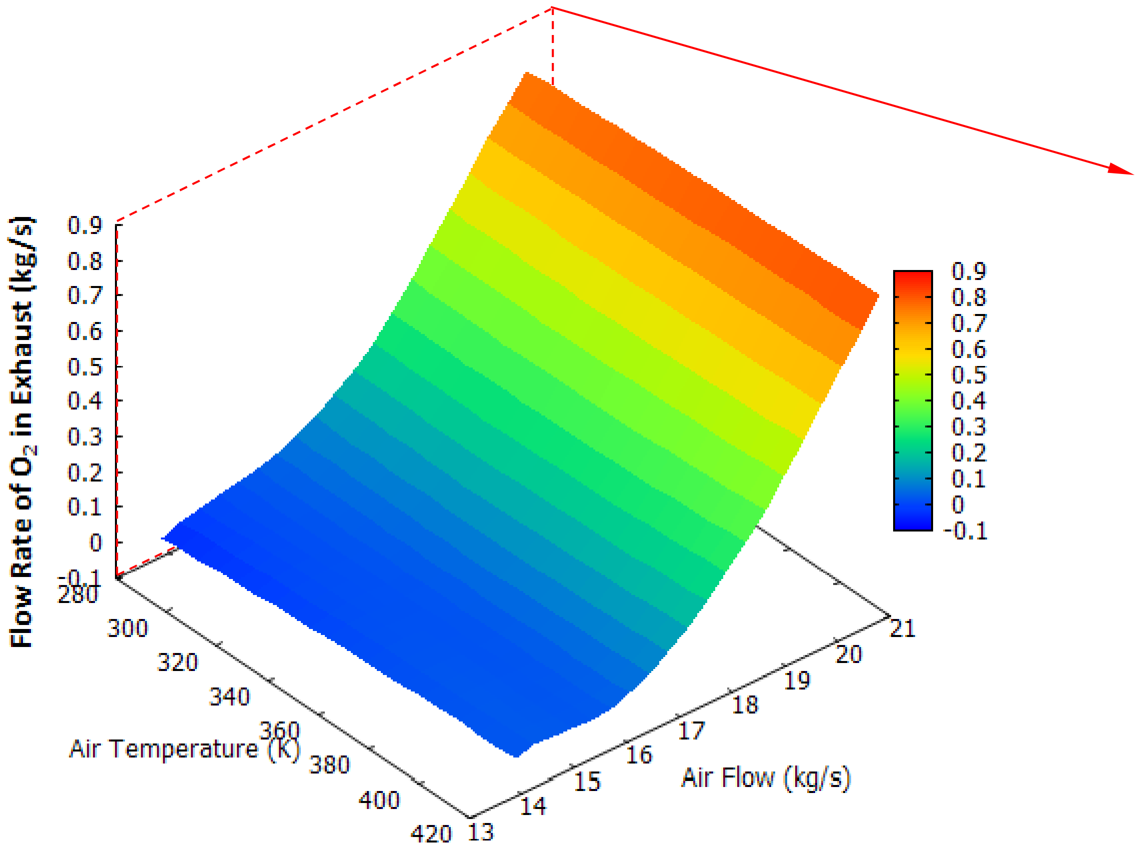
- **CH_4+Air→Products**
  - Const p, Adiabatic
  - Reactants: CH_4, O_2, N_2 (***m=3***)
  - Products: CH_4, O_2, N_2, H_2, H_2O, CO, CO_2, NO (***n=8***)
  - Elements: C, H, O, N (***l=4***)
  - High-Fidelity Model: **Aspen Plus**
- **Latin Hypercube Sampling (LHS)**
  - 10 samples
  - Two input variables T_{air}
    - ❖ Air Temperature $\dot{m}_{air}$
    - ❖ Air Mass Flow
- **Regression Method**
  - Kriging
  - ANN

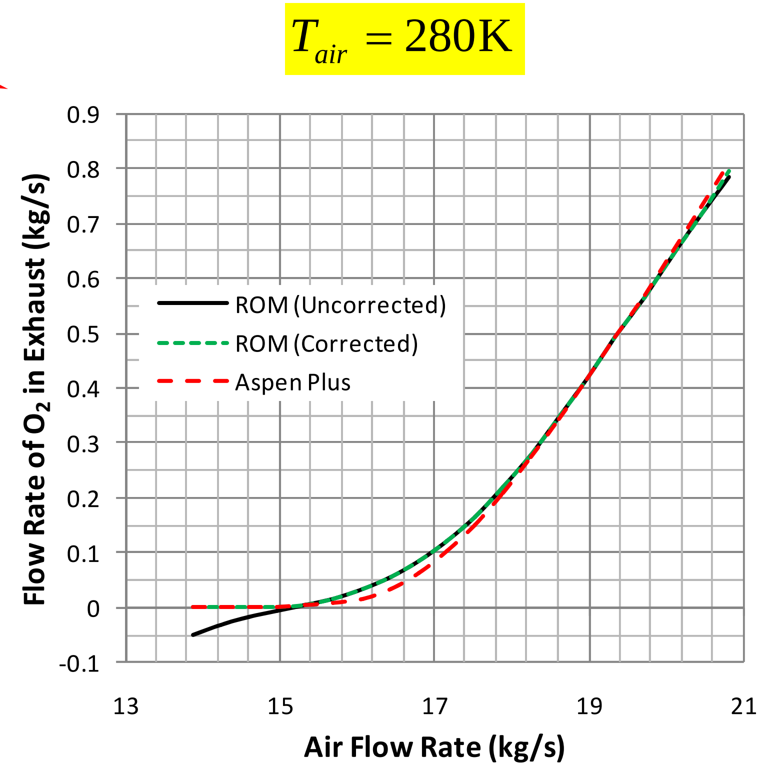




Example: Equilibrium Flow Reactor

Response Surface (Kriging)



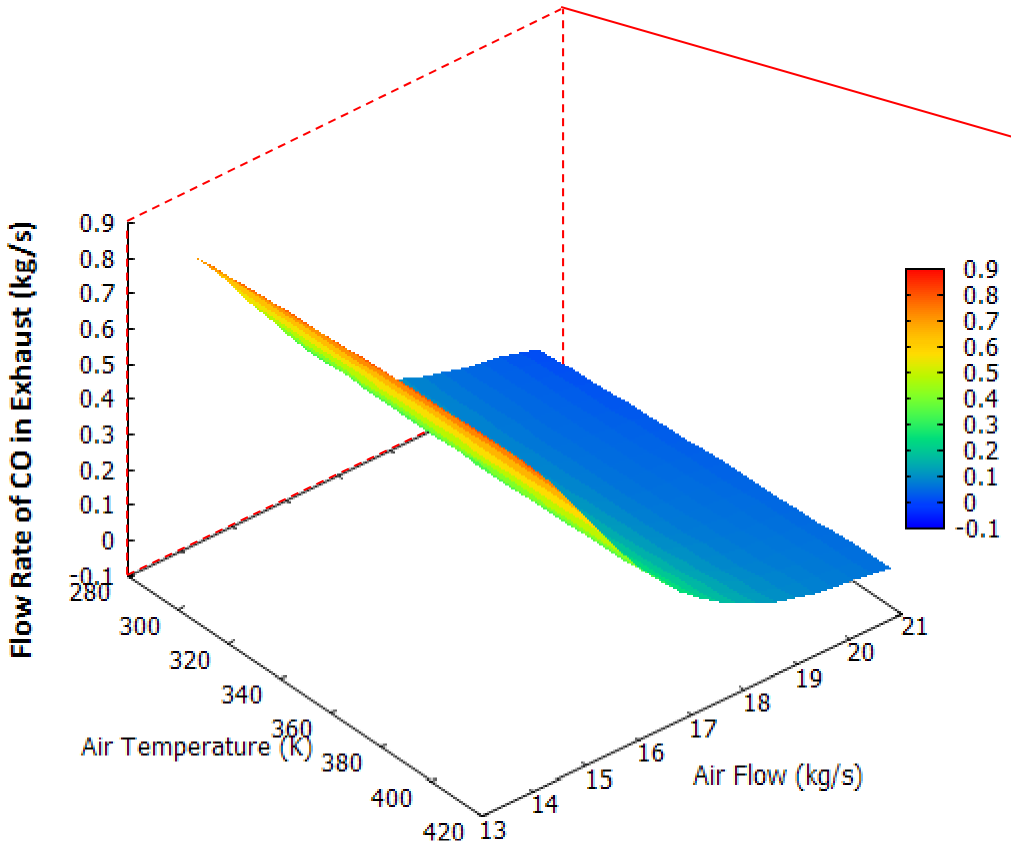


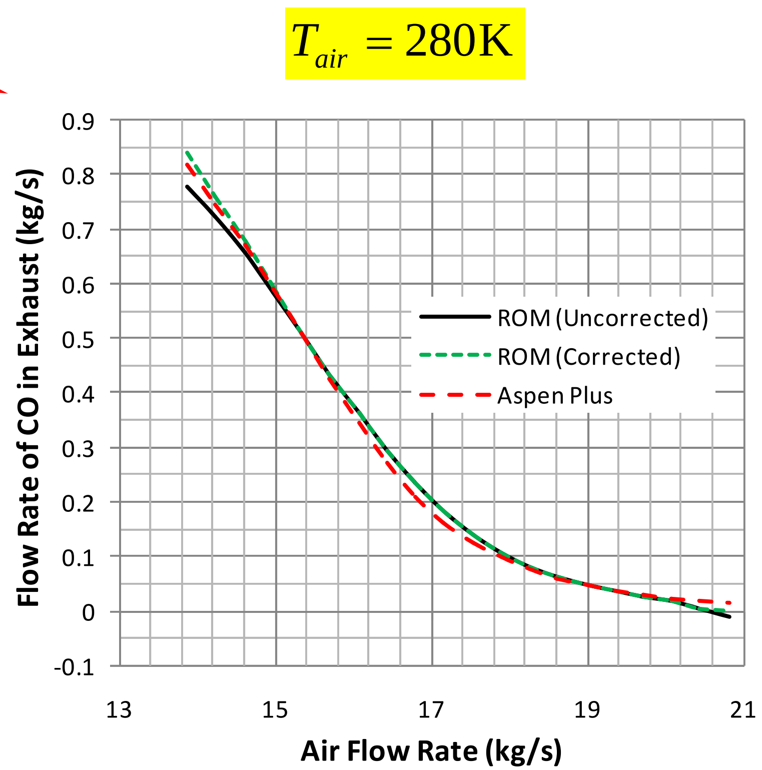
Flow rate of O_2 in exhaust versus air temperature and air flow rate

Flow rate of O_2 in exhaust versus air flow rate (280 K air temperature)

Example: Equilibrium Flow Reactor

Response Surface (Kriging)



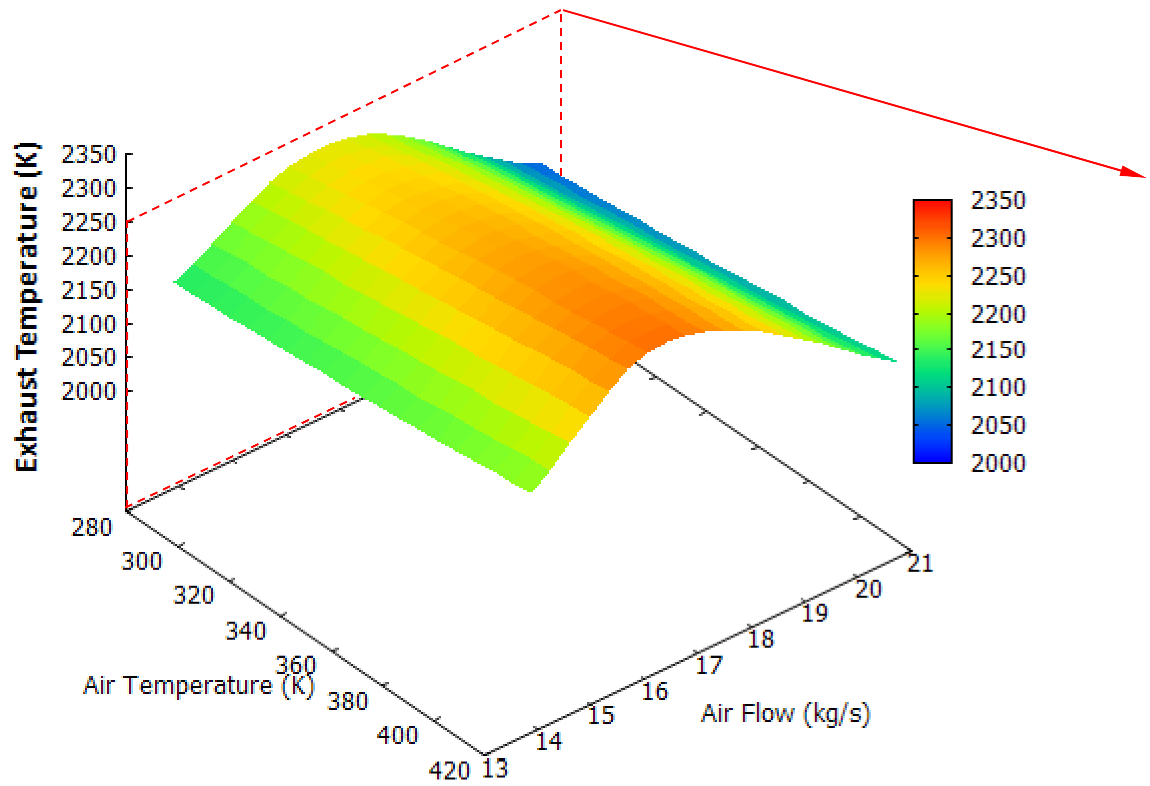


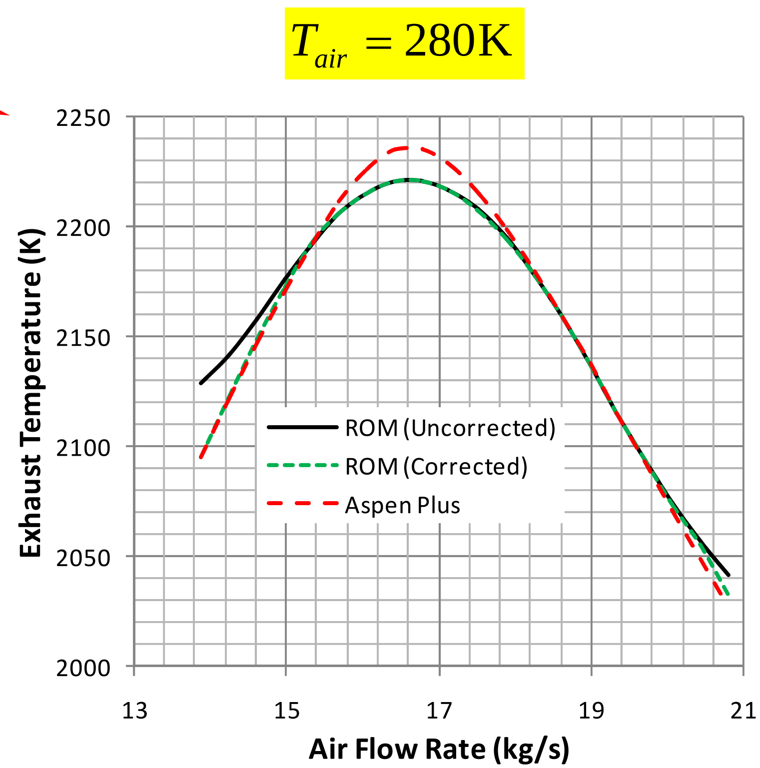
Flow rate of CO in exhaust versus air temperature and air flow rate

Flow rate of CO in exhaust versus air flow rate (280 K air temperature)

Example: Equilibrium Flow Reactor

Response Surface (Kriging)





Exhaust temperature versus air temperature and air flow rate

Exhaust temperature versus air flow rate (280 K air temperature)

Conclusions

- **Enforcing elemental mass balance for ROM**
  - Enforcing positive species flow rate
  - Lagrangian Multiplier Method (# of product species > # of elements)
  - Least Square Method (otherwise)
- **Enforcing energy balance**
  - Adjust heat loss
  - Adjust product enthalpy/temperature
- **Implementations**
  - CAPE-OPEN unit operation model
  - Custom model in ACM and gPROMS languages
- **Corrected ROM predictions are usually closer to high-fidelity model predictions**
  - Especially in regions with negative product flows predicted by ROM

Disclaimer

This presentation was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.