Enforcing Elemental Mass and Energy Balances for Reduced Order Models

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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

- **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

CO₂ Adsorber Model (CFD)

ROM

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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 $j$:  \[ \dot{L}_{j,in} = \sum_{i=1}^{m} \dot{N}_{i,in} A_{i,j} \quad \dot{L}_{j,out} = \sum_{i=1}^{n} \dot{N}_{i,out} A_{i,j} \]

Mass balance:  \[ \sum_{i=1}^{m} \dot{N}_{i,in} A_{i,j} = \sum_{i=1}^{n} \dot{N}_{i,out} A_{i,j} \quad (j=1,2,...,l) \]
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 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

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

Then

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

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
while enforcing mass balance for each element

$$\sum_{i=1}^{n} f_i^2$$

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

Lagrangian Function $G$:

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

Partial Derivatives of $G$:

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

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

Total number of equations: $n+l$
Total number of unknowns: $n+l$
Solving Correction Factors

Scenario 2: \( n < l \)

Example: \( \text{CO}_2 \) and \( \text{H}_2\text{O} \) as products (2 species, 3 elements)

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

\[
\sum_{i=1}^{n} \hat{N}_{i,\text{out}}^{\text{ROM}} A_{i,j} f_i = \Delta \hat{L}_j (j = 1, 2, \cdots, l) \quad \rightarrow \quad M\vec{f} = \vec{b} \quad \text{(Matrix } M \text{ is } l \times n )
\]

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

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

Total number of equations: \( n \)
Total number of unknowns: \( n \)

Note: Applicable to non-reacting devices
Enforcing Energy Balance

Stream Enthalpy:

\[ h_{\text{mix}}(T) = \sum_{k=1}^{s} y_k \left[ h^0_{f,k} + \int_{T_0}^{T} C_{p,k}(T')dT' \right] \]

(If ideal gas mixture)

Enthalpy Rate In:

\[ \dot{H}_{\text{in}} = \sum_{i=1}^{p} \dot{m}_{i,\text{in}} h_{i,\text{in}} \]

Enthalpy Rate Out:

\[ \dot{H}_{\text{out}} = \sum_{i=1}^{q} \dot{m}_{i,\text{out}} h_{i,\text{out}} \]

Energy Balance:

\[ \sum_{i=1}^{p} \dot{m}_{i,\text{in}} h_{i,\text{in}} = \sum_{i=1}^{q} \dot{m}_{i,\text{out}} h_{i,\text{out}} + \dot{W}_{\text{out}} + \dot{Q}_{\text{loss}} \]
Enforcing Energy Balance

Option 1: Adjusting heat loss

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

Option 2: Adjusting product stream enthalpy/temperature

Total Enthalpy Rate of Products:

\[ \dot{H}_{\text{out}} = \dot{H}_{\text{in}} - \dot{W}_{\text{out}} - \dot{Q}_{\text{loss}}^{\text{ROM}} \]

Total Enthalpy Rate Correction:

\[ \Delta \dot{H}_{\text{out}} = \dot{H}_{\text{out}} - \dot{H}_{\text{out}}^{\text{ROM}} = \dot{H}_{\text{in}} - \dot{W}_{\text{out}}^{\text{ROM}} - \dot{Q}_{\text{loss}} - \dot{H}_{\text{out}}^{\text{ROM}} \]

Enthalpy Rate Correction for Port \( i \):

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

Enthalpy Correction Per Unit Mass for Port \( i \):

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

Solve Temperature \( T_{i} \) for Port \( i \):

\[ \Delta h_{i,\text{out}} = \int_{T_{\text{ROM}}}^{T_{i}} C_{p,i}(T')dT' \quad \text{(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)
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$_2$O, 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 $T_{\text{air}}$, $\dot{m}_{\text{air}}$
    - Air Temperature $T_{\text{air}}$
    - Air Mass Flow $\dot{m}_{\text{air}}$
- **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)

$T_{air} = 280K$
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)

\( T_{air} = 280\text{K} \)
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)

\[ T_{air} = 280K \]
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
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