Reduced Order Models for Oxycombustion Boiler Optimization

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Project Objective

Develop an **equation oriented** framework to optimize a coal oxycombustion flowsheet.
Oxycombustion Flowsheet

1. Air Separation Unit
2. Boiler
3. Steam Turbine
4. Pollution Controls
5. CO₂ Compression Train
Boiler Design

• Economics of the power generation process depend strongly on optimized boiler performance
• Tight heat integration has been developed for traditional, air fired units
• Radiative heat transfer dominates
  • O₂ and CO₂ different properties than air
• Need detailed first principles model
Boiler Model

• Hybrid 1D reaction/3D radiation approach
• Reaction kinetics – considering particle size and composition
  • Boiler treated as vertical zones, each of which is a well mixed reactor
• Radiation – solved iteratively over a 3D mesh
  • 90% of heat transfer, convection is ignored in the radiative region
• Inlet stream properties → total heat transfer, outlet properties
Model Validation

• Geometries and operating conditions of two existing utility boilers
  • PacificCorp’s Hunter Unit 3

<table>
<thead>
<tr>
<th>Unit</th>
<th>Boiler Model</th>
<th>CFD Model</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enclosure Wall</td>
<td>$3.93 \times 10^8$</td>
<td>$4.03 \times 10^8$</td>
<td>2.4%</td>
</tr>
<tr>
<td>Platen</td>
<td>$9.89 \times 10^7$</td>
<td>$1.09 \times 10^8$</td>
<td>9.2%</td>
</tr>
</tbody>
</table>

• Trends in oxy vs. air-fired models match that of CFD simulations, e.g. higher burnout for oxy-fired boiler
Hybrid Model vs Full CFD Simulation
Reduced Order Models – Motivation

• Boiler model takes ~60 seconds to converge
• Iterative nature makes accurate derivatives difficult to obtain
• Construct simple algebraic representation (e.g. kriging), incorporate in equation oriented flowsheet
• Problem: How accurate should a ROM be to be useful for optimization? Can we ever find the optimum of the original detailed model?
Trust Region Framework - Introduction

- Allows us to carefully construct and update ROMs in a way that can guarantee convergence to a stationary point

\[ \min f(x, y) \quad \text{s.t.} \quad g(x, y) \leq 0, y = d(x) \]

- Consider the NLP:

\[ \psi(x) = f(x) + \nu \varphi(g(x)) \]

- Using penalty functions to handle the constraints, restate the problem as an unconstrained objective:
Trust Region Framework – Algorithm Outline

1) Given starting point \( x_0 \), construct ROM \( \psi^R \) around \( x_0 \)

2) Solve trust region subproblem:

\[
\min_s \psi^R(x_k + s), \quad \|x_k - s\| \leq \Delta_k
\]

3) Evaluate original detailed model at new step \( x_k + s \)

4) Adjust trust region radius \( \Delta_k \)

5) Go to 2)
Stopping Conditions

• Option 1: When gradient less than $\text{tol}_g$, enter criticality step
  • Systematically reduce TR around critical point until convergence or new improvement direction is found

• Option 2: $\epsilon$-exact termination – given an estimate $\epsilon$ of the error of the ROM over the trust region
  • Stop if optimization terminates within trust region and $\epsilon < \text{tol}_\epsilon$

$$\|x^* - \bar{x}\| \leq (2\bar{\sigma})^{3/2}(\epsilon)^{1/2}/(\sigma)^2$$
Conditions on Reduced Order Models

• The key to convergence is the fully linear property:

\[ |f(x) - f^r(x)| \leq \kappa_f \Delta^2, \quad \|\nabla f(x) - \nabla f^r(x)\| \leq \kappa_g \Delta \]
\[ \|g(x) - g^r(x)\| \leq \kappa_c \Delta^2, \quad \|\nabla g(x) - \nabla g^r(x)\| \leq \kappa_{gc} \Delta \]

• As trust region vanishes, function values and gradients approach original model

• Any type of ROM may be used satisfying this property
Optimization with Kriging Reduced Model

- Stage II has few degrees of freedom for optimization
- Easy to construct and validate an ε–exact Kriging approximation for Stage II model
Integrated Optimal Solution Comparison

Better solution is obtained with the integrated model

Improved computational efficiency over full 2-stage model

- 20% shorter batch time for integrated optimum
- Rigorous Optimum Verified
Conclusions

• Accurate representation of the boiler is essential for optimization of the oxy-combustion process
• Reduced order models allow optimization of flowsheets with complex black-box units
• Provably convergent trust region algorithms

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Kriging interpolation

- Given samples from Experimental design
- Choose linear basis of functions to fit with linear regression
- Exploit properties of Probability density function (assume white noise): Radial Basis Function (RBF), \( R(\theta, x) \). (Note Gaussian has \( p = 2 \))
- Optimize regression with respect to \( \theta \)
- Develop predictive model that combines linear regression model and RBF
- DACE MATLAB Toolbox (Lophaven et al., 2002)

**Predictor:**

\[
Y = F(x)\beta + r(x)\gamma
\]

\[
\beta^* = (F^T R^{-1} F)^{-1} F^T R^{-1} Y
\]

\[
\sigma^2 = \frac{1}{m} (Y - F\beta^*)^T R^{-1} (Y - F\beta^*)
\]

**Correlation function**

\[
R(\theta, x_i, x_j) = \prod_{k=1}^{nd} R_k(\theta, x_i^k - x_j^k)
\]

\[
R_k = \exp(-\theta_k |x_i^k - x_j^k|^p)
\]

\( \theta_k \): an indication of input correlation

1. \( \theta \neq \theta^L, \neq \theta^U \)
2. Small ratio of \( \max(\theta)/\min(\theta) \)
RM-based Trust Region Strategy without Gradients

Choose $\Delta_0$, $x_0$. Compute $\psi(x_0)$. Set $k=0$

Update ROM at $x_k$. Construct TR subproblem

Compute step $s_k$ that satisfies sufficient decrease condition for $\psi^R(x_k+s)$

$|D_x\psi^R| \leq \varepsilon$?

Yes

ROM fully linear?

Yes

STOP

No

Calculate $\psi(x_k+s_k)$ & $\rho_k = \text{ared/pred}$

No

Is $\rho_k \geq \eta_k$?

Yes

$x_{k+1} = x_k + s_k$

Update $\Delta_k$

No

$\Delta \leq \varepsilon$?

Yes

STOP

No

Shrink $\Delta_k$

$\text{ROM fully linear?}$

Yes

STOP

No

Case Study: Semi-Interpenetrating Polymer Network (SIPN)

0. Swelling

I. Polymerization.

II. Crosslinking

Particle Growth Model (make)

Semi-IPN Kinetic Model (bake)

Integrated Optimization

- Include both models into optimization

New optimization problem formulation

\[
\begin{align*}
\min_{v^l, v^u} & \quad t_I + t_{II} \\
\text{s.t.} & \quad \text{stage I model} \\
& \quad \text{Stage II surrogate model:} \\
& \quad \{ Gel_{end} = S_1(v^{II}_c); \} \\
& \quad \{ \bar{M}w_{end} = S_2(v^{II}_c) \} \\
& \quad Gel_{end} \geq Gel_{tar} \\
& \quad \bar{M}w_{end} \geq \bar{M}w_{tar} \\
& \quad v^l_I \leq v^u_c \leq v^u_I \\
& \quad v^l_{II} \leq v^u_c \leq v^u_{II}
\end{align*}
\]

- Minimize overall reaction time
- Subject to Rigorous Stage I model & Kriging Stage II model
- Consider final property constraints
- Control bounds