Dynamic Optimization in the Process Industry – Application Studies

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Outline

- Introduction
- Design for operability
- Optimal response under partial plant shutdown
- Dynamic optimization of electric arc furnace (EAF) operation
- Concluding remarks

Introduction

- Focus on 3 industrial application studies involving DAE optimization conducted through the
  - McMaster Advanced Control Consortium (MACC)
  - McMaster Steel Research Centre (SRC)
- Applications are different in nature and span different industrial sectors – chemical, pulp & paper, and steel.
- Overview of objectives, formulation & solution, and specific challenges.

Design for Dynamic Operability

- The design of a plant can significantly affect its dynamic performance.
- Plants are traditionally designed on basis of steady-state considerations, with control system designed in a subsequent step.
- Plants with poor dynamics characteristics may result in failure to
  - meet product quality specifications
  - achieve expected economic performance
  - satisfy safety and environmental constraints
- Motivates need for systematic framework for addressing dynamic performance considerations at plant design stage.
- Optimization-based approaches consider performance-limiting factors simultaneously, and offer considerable flexibility in problem formulation.

Integrated Design Formulation

$$\min_{\mathbf{d}} \quad \underset{\theta(\mathbf{t})\in\Gamma}{\mathrm{E}} \{\Phi[\mathbf{d}, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}(t)]\}$$

$$\begin{aligned} \text{subject to:} \quad \mathbf{h}[\,\mathbf{d}, \dot{\mathbf{x}}(t), \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}(t), t\,] &= 0 \\ \mathbf{g}[\,\mathbf{d}, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}(t), t\,] &\leqslant 0 \\ \mathbf{x}(0) &= \mathbf{x}_0 \\ t &= [\,0, t_f\,] \\ \boldsymbol{\theta}(t) &= \Gamma \end{aligned}$$

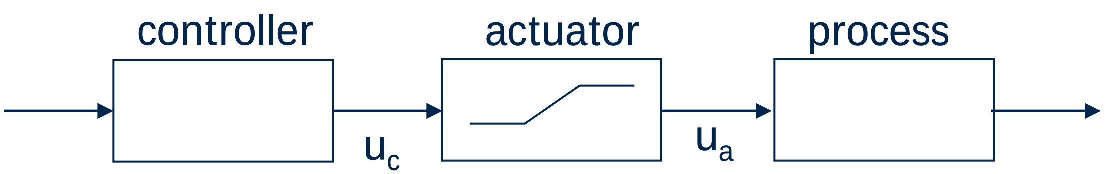
$$\text{where:} \quad \Gamma = \{\,\boldsymbol{\theta}(t), \boldsymbol{\theta}^L(t) \leqslant \boldsymbol{\theta}(t) \leqslant \boldsymbol{\theta}^U(t)\,\}$$

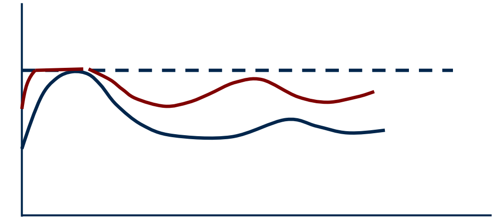
$$\begin{aligned} \mathbf{d} &= \text{design variables} \\ \mathbf{x}(t) &= \text{state variables} \\ \mathbf{u}(t) &= \text{manipulated inputs} \\ \boldsymbol{\theta}(t) &= \text{uncertain parameters} \end{aligned}$$

Remarks

- Uncertainty typically handled using multiperiod formulation.
- Could consider open- or closed-loop response.
- Design variables may include equipment sizing, steady-state operating point, controller tuning parameters and structural decisions (control structure, plant configuration)
- *Prior work by our group: formulation of model discontinuities associated with controller output.*

Actuator Saturation





Logical description

$$u_a(k) = \begin{cases} u_L & u_c(k) \le u_L \\ u_c(k) & u_L \le u_c(k) \le u_U \\ u_U & u_c(k) \ge u_U \end{cases}$$

Complementarity constraint formulation

$$u_c(k) = u_a(k) - S_L(k) + S_U(k)$$

$$0 = S_L(k)(u_a(k) - u_L)$$

$$0 = S_U(k)(u_a(k) - u_U)$$

$$0 \le S_L(k)$$

$$0 \le S_U(k)$$

$$u_L \le u_a(k) \le u_U$$

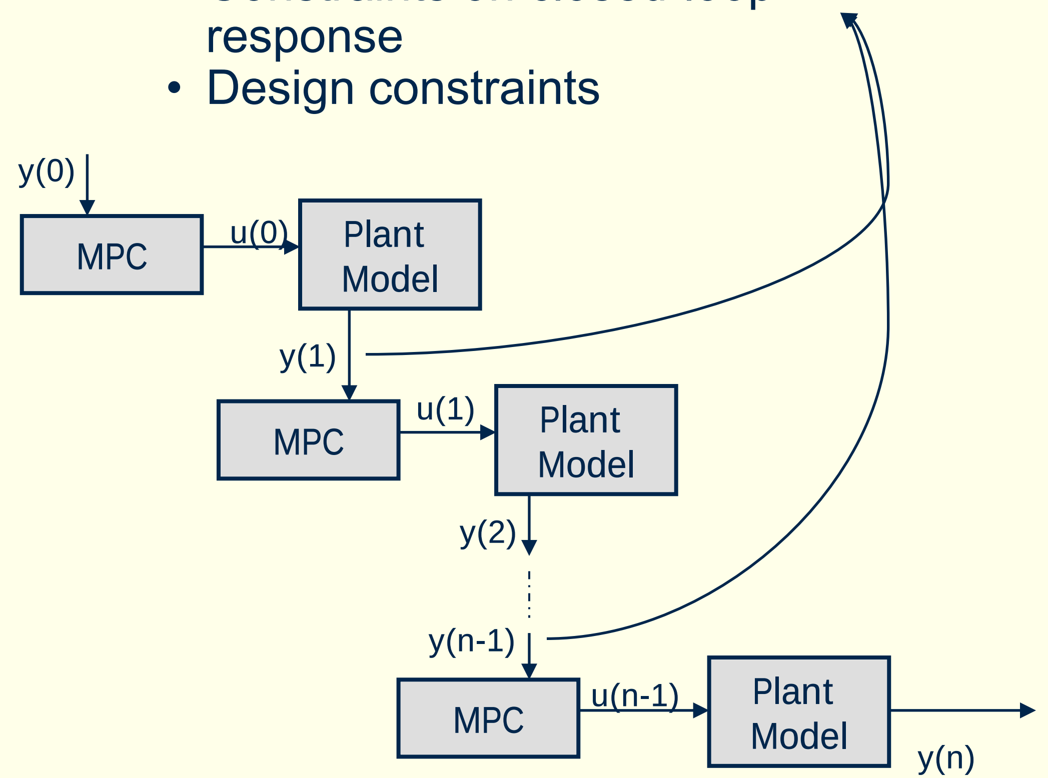
Constrained MPC as Plant Controller

- Sequence of:
  - controller optimization subproblems and
  - model simulations

  within primary dynamic optimization

- Simultaneous solution approach followed to:
  - avoid derivative discontinuities associated with constrained MPC.
  - avoid difficulties with potential closed-loop instability.

Min Φ
Subject to:
- Constraints on closed-loop response
- Design constraints



Reformulation as MPCC

- Reformulation permitted by convexity of MPC QPs.
- Replace MPC quadratic programming (QP) subproblems with their Karush-Kuhn-Tucker (KKT) conditions.

QP

$$\min_{\mathbf{x}} \frac{1}{2}\mathbf{x}^T H\mathbf{x} + \mathbf{g}^T\mathbf{x}$$
$$s.t. \quad A\mathbf{x} = \mathbf{b}$$
$$\mathbf{x} \geq \mathbf{0}$$

KKT

$$\left.\begin{aligned} H\mathbf{x} - A^T\mathbf{v} + \mathbf{g} - \mathbf{u} &= \mathbf{0} \\ A\mathbf{x} &= \mathbf{b} \end{aligned}\right\} \text{linear}$$
$$u_i x_i = 0$$
$$(\mathbf{u}, \mathbf{x}) \geq \mathbf{0}$$

complementarity

- Gives rise to single-level mathematical program with complementarity constraints (MPCC).

Solution – I. Interior-Point Approach

$$\begin{aligned} & \min \ \phi(\mathbf{x}, \mathbf{y}, \mathbf{z}) \\ \text{subject to} \quad & \mathbf{h}(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{x}, \mathbf{y}, \mathbf{z}) \geq \mathbf{0} \\ & c_i(\mathbf{x}, \mathbf{y}) = x_i y_i \\ & \qquad = 0 \qquad \forall\, i = 1, 2, \ldots, n_c \\ & (\mathbf{x}, \mathbf{y}) \geq \mathbf{0} \end{aligned}$$

Lagrangian

$$\mathcal{L}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \boldsymbol{\lambda}, \boldsymbol{\theta}, \boldsymbol{\rho}, \boldsymbol{\pi}, \boldsymbol{\psi}) = \phi(\mathbf{x}, \mathbf{y}, \mathbf{z}) - \boldsymbol{\lambda}^T \mathbf{h}(\mathbf{x}, \mathbf{y}, \mathbf{z}) - \boldsymbol{\theta}^T \mathbf{g}(\mathbf{x}, \mathbf{y}, \mathbf{z}) - \boldsymbol{\rho}^T \mathbf{c}(\mathbf{x}, \mathbf{y}) - \boldsymbol{\pi}^T \mathbf{x} - \boldsymbol{\psi}^T \mathbf{y}$$

Remarks

1. Complementarity constraints separated from general equality constraints.
2. Variable set partitioned into (x,y,z) with x,y appearing in complementarity constraints.

KKT Conditions

$$\begin{aligned}
\nabla_{\mathbf{x}}\mathcal{L} = \nabla_{\mathbf{x}}\phi(\mathbf{x},\mathbf{y},\mathbf{z}) - H_{\mathbf{x}}^{T}(\mathbf{x},\mathbf{y},\mathbf{z})\,\boldsymbol{\lambda} - G_{\mathbf{x}}^{T}(\mathbf{x},\mathbf{y},\mathbf{z})\,\boldsymbol{\theta} - C_{\mathbf{x}}^{T}(\mathbf{x},\mathbf{y})\,\boldsymbol{\rho} - \boldsymbol{\pi} = \mathbf{0} \\
\nabla_{\mathbf{y}}\mathcal{L} = \nabla_{\mathbf{y}}\phi(\mathbf{x},\mathbf{y},\mathbf{z}) - H_{\mathbf{y}}^{T}(\mathbf{x},\mathbf{y},\mathbf{z})\,\boldsymbol{\lambda} - G_{\mathbf{y}}^{T}(\mathbf{x},\mathbf{y},\mathbf{z})\,\boldsymbol{\theta} - C_{\mathbf{y}}^{T}(\mathbf{x},\mathbf{y})\,\boldsymbol{\rho} - \boldsymbol{\psi} = \mathbf{0} \\
\nabla_{\mathbf{z}}\mathcal{L} = \nabla_{\mathbf{z}}\phi(\mathbf{x},\mathbf{y},\mathbf{z}) - H_{\mathbf{z}}^{T}(\mathbf{x},\mathbf{y},\mathbf{z})\,\boldsymbol{\lambda} - G_{\mathbf{z}}^{T}(\mathbf{x},\mathbf{y},\mathbf{z})\,\boldsymbol{\theta} = \mathbf{0}
\end{aligned}$$

$$\begin{aligned}
\mathbf{h}(\mathbf{x},\mathbf{y},\mathbf{z}) &= \mathbf{0} \\
\mathbf{g}(\mathbf{x},\mathbf{y},\mathbf{z}) - \mathbf{u} &= \mathbf{0} \\
x_i y_i &= 0 && \forall\, i = 1,\ldots,n_c \\
\pi_i x_i &= 0 && \forall\, i = 1,\ldots,n_c \\
\psi_i y_i &= 0 && \forall\, i = 1,\ldots,n_c \\
\theta_i u_i &= 0 && \forall\, i = 1,\ldots,n_g \\
(\mathbf{x},\mathbf{y},\boldsymbol{\theta},\boldsymbol{\pi},\boldsymbol{\psi},\mathbf{u}) &\geq \mathbf{0}
\end{aligned}$$

where K_j is the Jacobian of the set of functions k with respect to the vector of variables j.

Solve via Newton iterates with relaxed complementarity constraints

$$\begin{aligned} x_i y_i &= 0 \\ \pi_i x_i &= 0 \\ \psi_i y_i &= 0 \\ \theta_j u_j &= 0 \end{aligned} \quad \longrightarrow \quad \begin{aligned} x_i y_i &= \mu \\ \pi_i x_i &= \mu \\ \psi_i y_i &= \mu \\ \theta_j u_j &= \mu \end{aligned} \qquad \begin{aligned} i &= 1,2,\ldots,n_c \\ j &= 1,2,\ldots,n_g \end{aligned}$$

where

$$\mu = \frac{\sigma}{3n_c + n_g}\left(\sum_{i=1}^{n_c} x_i y_i + \pi_i x_i + \psi_i y_i + \sum_{j=1}^{n_g} \theta_i u_i\right)$$

$$0 < \sigma < 1$$

Remark

Developed own implementation[1], but later switched to IPOPT-C[2].

[1]Baker, R. and C.L.E Swartz, MOPTA, 2001

[2]Raghunathan, A. U. and L. T. Biegler, *Comp. and Chem. Eng.* , 27:1381-1392, 2003

Solution – II. Penalty Approach

MPCC

$$\begin{aligned} \min \quad & \phi(\mathbf{x},\mathbf{y},\mathbf{z}) \\ \text{s.t.} \quad & \mathbf{h}(\mathbf{x},\mathbf{y},\mathbf{z}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{x},\mathbf{y},\mathbf{z}) \geq \mathbf{0} \\ & c_i(x_i, y_i) = x_i y_i = 0, \quad i = 1, 2, ..., n_c \\ & (\mathbf{x},\mathbf{y}) \geq \mathbf{0}, \end{aligned}$$

Reformulation

$$\begin{aligned} \min \quad & \phi(\mathbf{x},\mathbf{y},\mathbf{z}) + \mu \sum_{i=1}^{n_c} x_i y_i \\ \text{s.t.} \quad & \mathbf{h}(\mathbf{x},\mathbf{y},\mathbf{z}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{x},\mathbf{y},\mathbf{z}) \geq \mathbf{0} \\ & (\mathbf{x},\mathbf{y}) \geq \mathbf{0}, \end{aligned}$$

Remarks

- Exact penalty formulation. Convergence properties presented in Ralph and Wright[‡].
- Reformulated MPCC solved using NLP solver, IPOPT.

[‡] Ralph, D. and S.J. Wright, *Optimization methods and Software*, 19(5), 527-556, 2004.

Solution – III. MIP Approach

Solution as mixed-integer program

$$u_i x_i = 0 \longrightarrow \boxed{\begin{array}{l} 0 \le u_i \le (1 - z_i)\beta \\ 0 \le x_i \le z_i\beta \\ z_i \in \{0,1\} \end{array}}$$

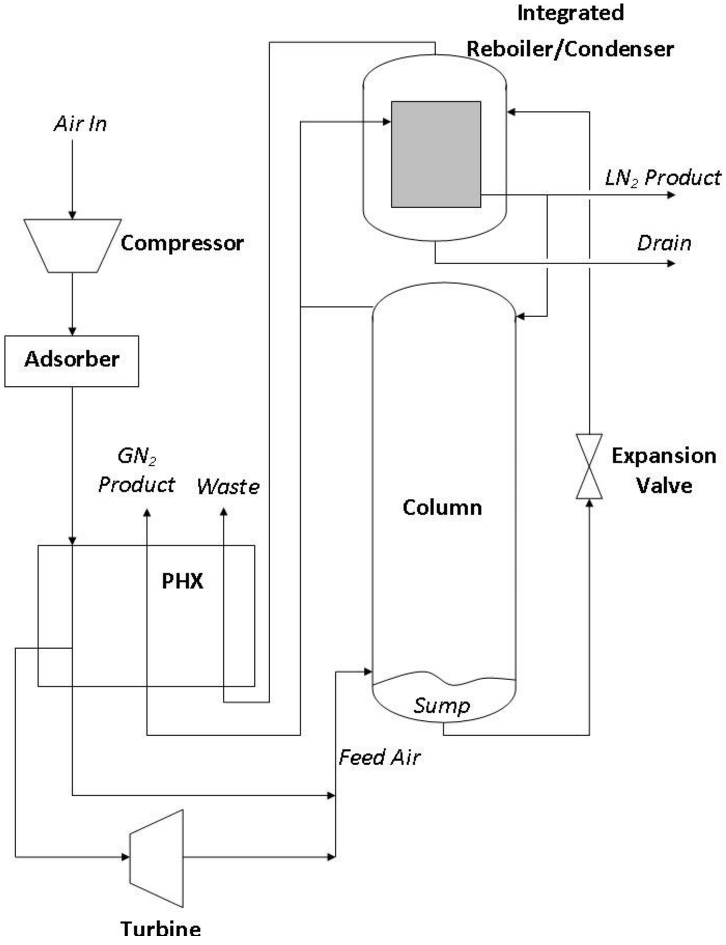
Remarks

- Global optimality guaranteed for a class of MIQPs we considered.
- Found to be significantly slower than both interior-point and penalty formulations.
- Interior-point approach consistently found global optimum when outer subproblem is quadratic with linear constraints.

Design for Fast Transitions

Motivation and Objectives

- Cryogenic air separation is a large consumer of electrical energy.
- Responsiveness to electricity price fluctuations and variations in customer demand would yield significant economic benefit.
- Dynamic optimization provides useful framework for assessment of design limitations to agility.
- Provides a benchmark for control performance.
- *Collaboration with Praxair Inc.*



Air Separation Unit (ASU) Model – I

Distillation

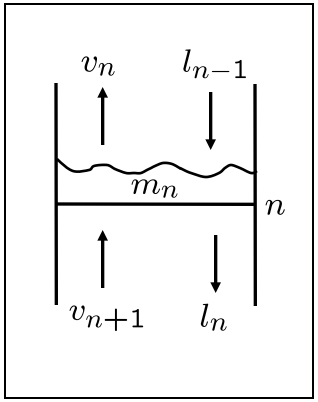
Material balances

$$\frac{dm_{n,i}}{dt} = l_{n-1,i} + v_{n+1,i} - l_{n,i} - v_{n,i}$$

Composition

$$l_{n,i} = x_{n,i}L_n \qquad L_n = \sum_{i=1}^{c} l_{n,i}$$

$$v_{n,i} = y_{n,i}V_n \qquad V_n = \sum_{i=1}^{c} v_{n,i}$$



Energy balances

$$\frac{dE_n}{dt} = H^{liq}_{n-1} + H^{vap}_{n+1} - H^{liq}_{n} - H^{vap}_{n}$$

$$E_n = \sum_{i=1}^{c} m_{n,i}h^{liq}_{n,i}$$

$$H^{liq}_n = \sum_{i=1}^{c} l_{n,i}h^{liq}_{n,i}$$

$$H^{vap}_n = \sum_{i=1}^{c} v_{n,i}h^{vap}_{n,i}$$

Equilibrium

$$y^{equil}_{n,i} = K_{n,i}x_{n,i}$$

$$K_{n,i} = \frac{\gamma_{n,i}P^{sat}_{n,i}}{P_n}$$

$$\ln(P^{sat}_{n,i}) = A_i + \frac{B_i}{T_n + C_i}$$

Tray hydraulics

$$M_n = A_s\rho^{liq}_n[H_{weir} + 1.41(\frac{L_n}{\sqrt{g}\rho^{liq}_n L_{weir}})^{2/3}]$$

Efficiency

$$y_{n,i} = y_{n+1,i} + \eta_n(y^{equil}_{n,i} - y_{n+1,i})$$

Remarks

- Direct formulation results in index-2 DAE system.
- Manual index reduction performed.

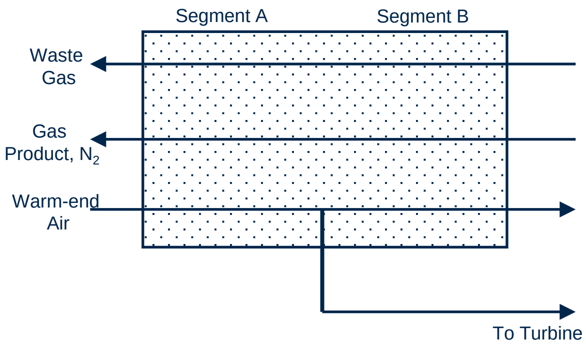
Air Separation Unit (ASU) Model – II

Primary Heat Exchanger

- Approximated as series of perfectly mixed compartments.
  distributed parameter → lumped parameter system
- Model comprises differential energy balances, heat transfer relationships, and flow-dependent heat transfer coefficients

Compressor and Turbine

- Empirical: developed based on given compressor map.
- System of algebraic equations.



Composite Plant Model

- Unit models assembled into plant configuration
- Parameter estimation performed using plant operating and design data.
- Relative percent errors less than 1%.
- Coded and solved using gPROMS/gOPT.

Optimization Formulation

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Two-tiered approach

- **First** - solve a constrained ***steady-state optimization*** problem to determine an ***economically optimal*** target operating point.

$$\max_{\mathbf{u},F_{evap}} \Phi_{ss} = C_{GN_2}(F_{GN2,prod}+F_{evap})-(C_{comp}W_p+C_{evap}F_{evap})$$

subject to

$$\begin{aligned} \mathbf{f}(\dot{\mathbf{x}}=\mathbf{0},\mathbf{x},\mathbf{z},\mathbf{u},\mathbf{p}) &= \mathbf{0} \\ \mathbf{g}(\mathbf{x},\mathbf{z},\mathbf{u},\mathbf{p}) &= \mathbf{0} \\ \mathbf{h}(\mathbf{x},\mathbf{z},\mathbf{u},\mathbf{p}) &\leq \mathbf{0} \end{aligned}$$

- **Then** - solve a dynamic optimization problem to determine the optimal transition to the new steady-state..

$$\min_{\mathbf{u}(t),t_f} \Phi = t_f\{\int_{t_0}^{t_f}(1-\frac{F_{GN2,prod}}{F^*_{GN2,prod}})^2 dt+\sum_{i=1}^{N_u} w_i[1-\frac{u_i(t_f)}{u_i^*}]^2\}$$

subject to

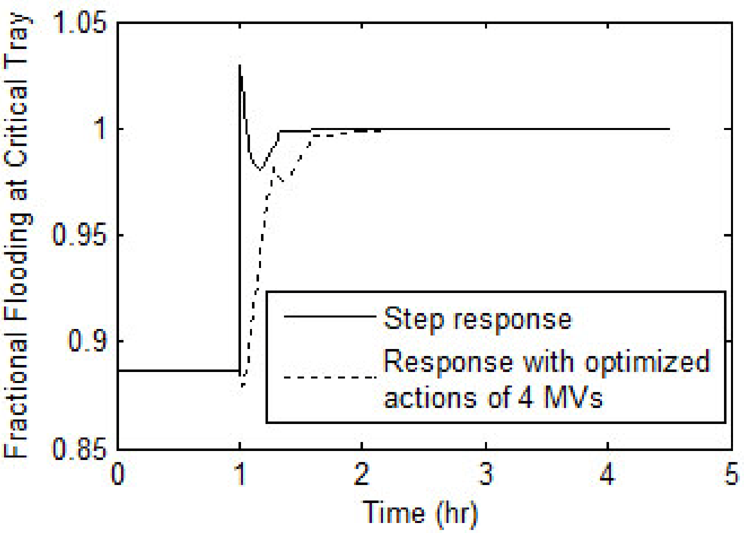
model equations and operational constraints

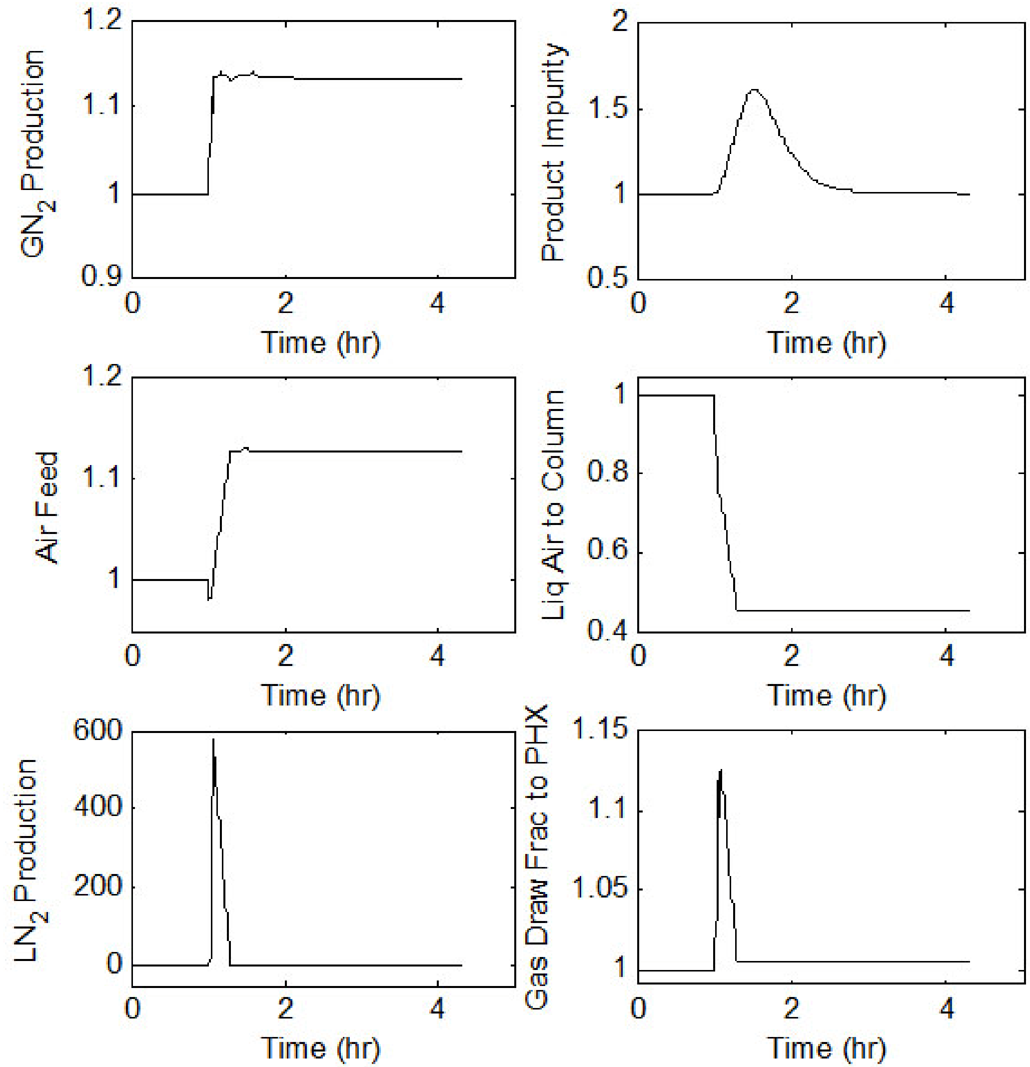
Dynamic Optimization Results

Setup:

- 20 % demand increase
- Change in demand at t = 1 hr

- First, performed dynamic simulation with step changes applied to inputs.
- Column flooding constraint violated – motivates necessity for dynamic optimization





Design Study: Introducing External LN2

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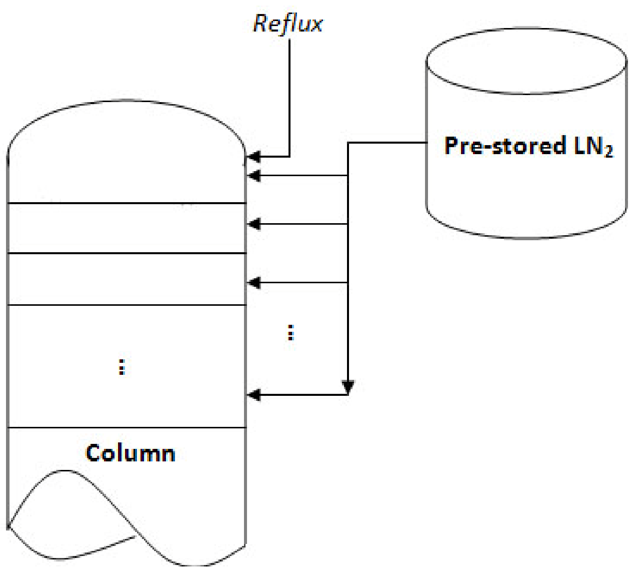
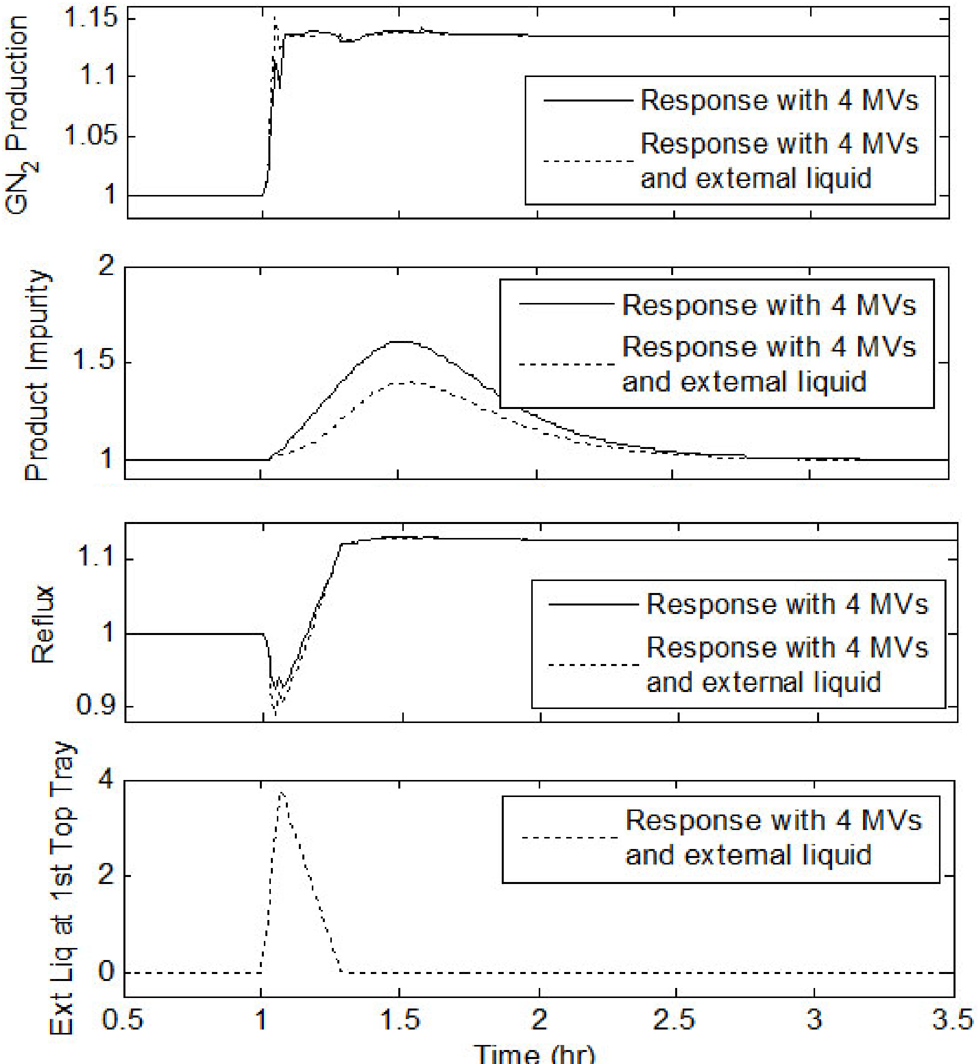
- Allow introducing pre-stored liquid nitrogen into the column during transition for cases where flooding constraint may be active.
- Example: 20 % demand increase



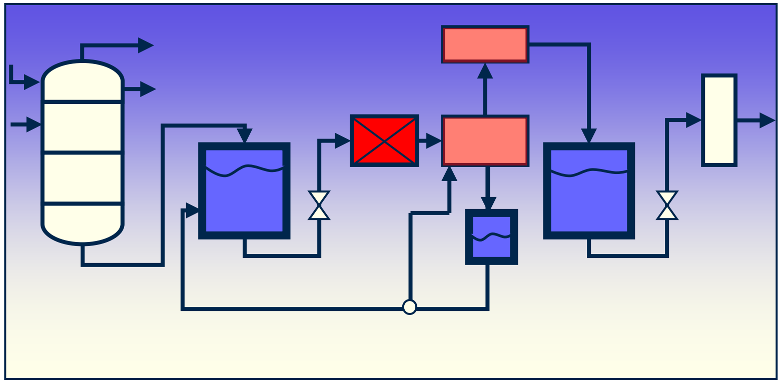


Remarks

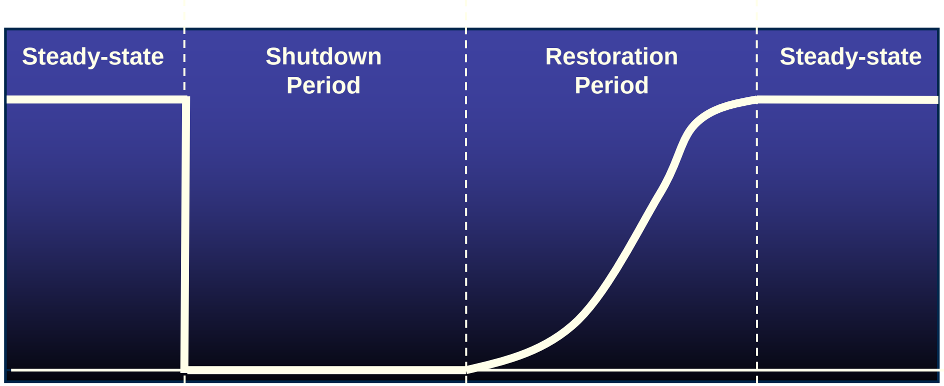
- Numerically challenging:
  - strongly nonlinear
  - tight thermal integration of subsystems
  - relatively high dimension (~ 550 differential, 6,900 algebraic variables)
  - discontinuous enthalpy relationships
- Highly sensitive to:
  - initialization
  - variable scaling & transformation
  - error control and optimization tolerances
- Future directions
  - Inclusion of design parameters as decision variables
  - 3-column plant
  - DAE optimization methodologies for large-scale, highly nonlinear, mixed-integer dynamic optimization problems

Dynamic Optimization under Partial Plant Shutdown

- **Partial shutdown** = unit shutdown that does not shut down the entire plant.
- Aim is to find a set of control actions that will:
  - keep rest of the plant operational (to some degree).
  - maximize economics.
  - satisfy safety and operational constraints.
- Means used to achieve this:
  - Buffer tanks to decouple departments.
  - Manipulating production rates and recycles.
  - Others: reconfiguring process pathways, employing redundancies, etc.



Collaboration with Tembec



Production through Unit vs Time

Dynamic Optimization Formulation

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$$\max_{\mathbf{u}(t)} \Phi_{economics}$$

subject to

Economics-based Objective Function

$$\Phi_{economics} = \sum_{m \in K} \left[C_m \int_0^{t_f} F_m \, dt \right] \qquad (1)$$

Model Equations and Constraints

$$\mathbf{f}(\dot{\mathbf{x}}(t), \mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), t) = \mathbf{0} \qquad (2)$$

$$\mathbf{g}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), t) = \mathbf{0} \qquad (3)$$

$$\mathbf{h}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), t) \leq \mathbf{0} \qquad (4)$$

for $t \in [0, t_f]$

Variable bounds

$$\mathbf{x_L} \leq \mathbf{x}(t) \leq \mathbf{x_U} \qquad (5)$$

$$\mathbf{z_L} \leq \mathbf{z}(t) \leq \mathbf{z_U} \qquad (6)$$

$$\mathbf{u_L} \leq \mathbf{u}(t) \leq \mathbf{u_U} \qquad (7)$$

for $t \in [0, t_f]$

Initial conditions

$$\mathbf{x}(0) = \mathbf{x}_0 \qquad (8)$$

Restoration constraints

$$\mathbf{x}_0 - \epsilon_x \leq \mathbf{x}(t) \leq \mathbf{x}_0 + \epsilon_x \quad \text{for } t_{res} < t \leq t_f \qquad (9)$$

$$\mathbf{u}_0 - \epsilon_u \leq \mathbf{u}(t) \leq \mathbf{u}_0 + \epsilon_u \quad \text{for } t_{res} < t \leq t_f \qquad (10)$$

Shutdown constraints

$$F_{in,unit}(t) = f_{shutdown} \quad \text{for } t_{start} \leq t \leq t_{end} \qquad (11)$$

- Dynamic model of plant in Differential-Algebraic-Equation (DAE) form.
- Solution method
  - Full discretization simultaneous strategy.
  - Modeled using in-house modeling language, MLDO.
  - IPOPT interior point solver used.
- Restoration constraints
  - Forces system to return to original steady-state once shutdown is over.
- Shutdown
  - Modeled by turning off flows to the shut down unit.

Approach to Nonunique Trajectories

- **Non-unique trajectories** arise frequently from economic objectives
  - Different control strategies give rise to same optimal objective value.
  - Manifest in chatter-like input trajectories. Undesirable for implementation.
- **Two-tiered optimization** (hierarchical optimization)
  - Solve the nonlinear program in two phases.

Tier 1: Economic optimization

$$J^*_{economics} = \max_{\mathbf{u}} \Phi_{economics}$$

Tier 2: Minimize control effort

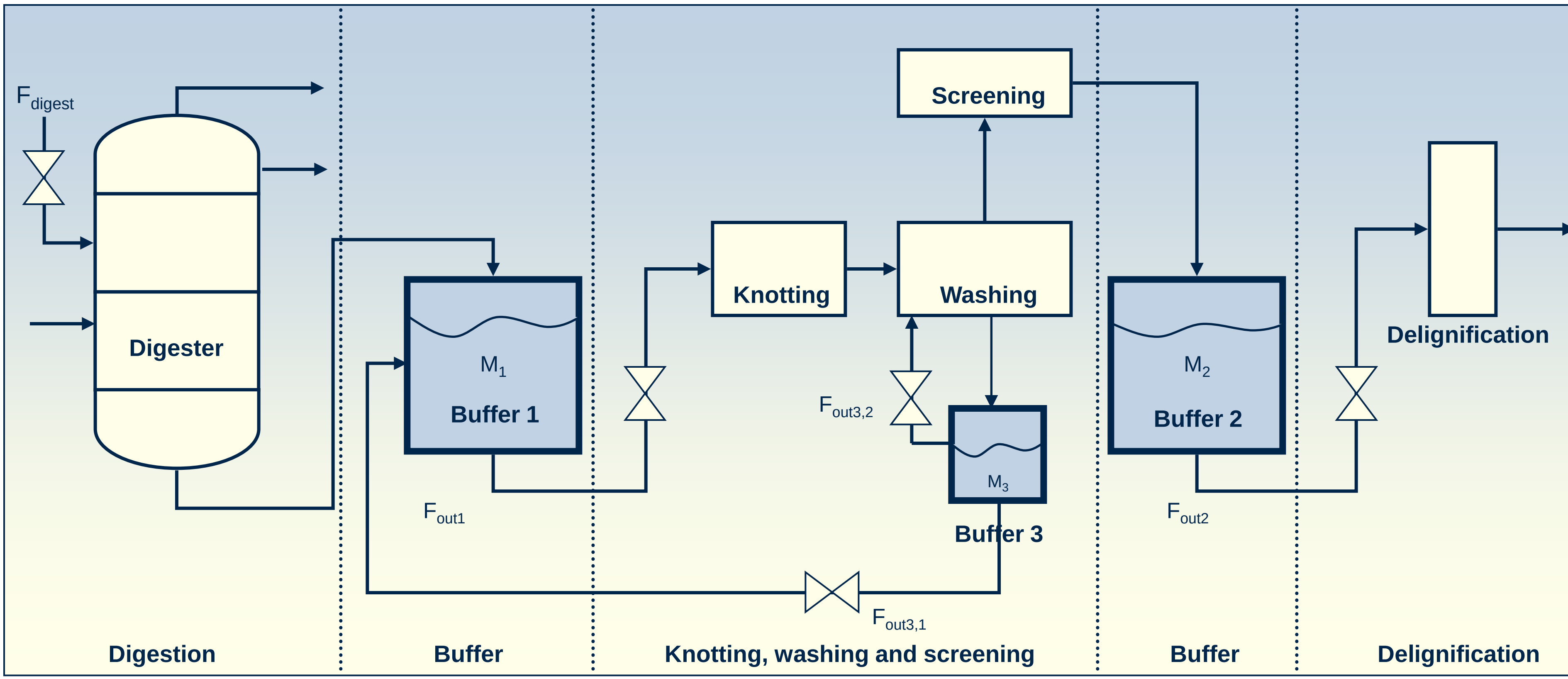
$$\begin{aligned} & \min_{\mathbf{u}} ||\Delta \mathbf{u}||_2 \\ \text{s.t.} \quad & \Phi_{economics} \geq (1-\xi) \cdot J^*_{economics} \end{aligned}$$

where ξ = percentage of original economics the customer is willing to trade off to obtain a smoother trajectory (commonly set to 1%).

  - Obtain trajectories that require **minimum control effort** to achieve specified level of **economic performance**.

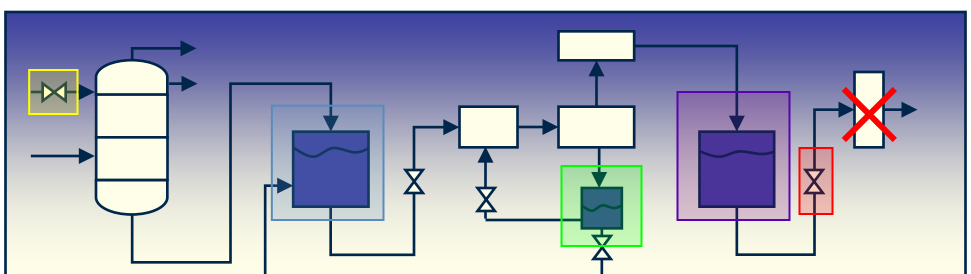
Case Study: Kraft Pulp & Paper Plant

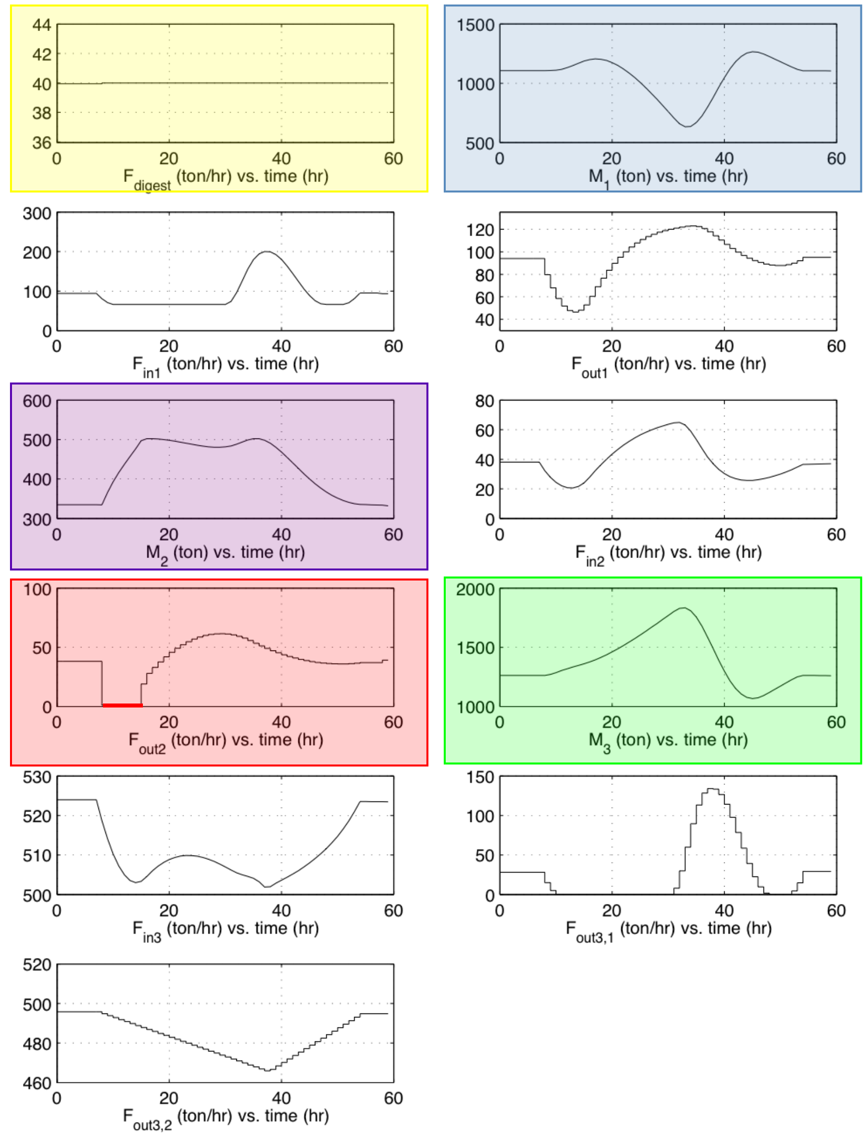
- Collaboration with pulp and paper company in Temiscaming, Québec.
- Fiber line process: 5 departments, 3 dynamic buffer units, 2 recycles.
- Pseudo-steady-state assumption for non-dynamic units.
- Units shut down from time to time, for maintenance or due to failure.



Case: Delignification Shutdown

- Shutdown in delignification department (8-14 hrs)
- Calculate optimal open-loop control policies for controlling plant. Two-tiered optimization.
- Results:
  - Digester at maximum production.
  - Buffer 1 contents discharged to make up for lost production.
  - Buffer 2 accumulates product and discharges contents during restoration phase.





Modeling Language for Dynamic Optimization (MLDO)

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$$\max_{U} \; [1 - z_a - z_b]$$

$$s.t.$$

$$\frac{dz_a}{dL} = U(10 z_b - z_a)$$

$$0 \leq U \leq 1$$

Mathematical description

```
minimize: -(1 - za(tf_) -
zb(tf_));
dae:
$za = U*(10*zb - za);
constraints: 0 <= U <= 1;
...
```

One representation…

- Simple math-like language to describe dynamic optimization problems.
- Generates code in many languages.
- Written in Python. Currently used as a research tool for rapid prototyping.

DAE Model in MLDO

$$\min_{\mathbf{u}(t),\boldsymbol{\theta}} \Phi(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \boldsymbol{\theta}, t_f)$$

$$\mathbf{f}(\mathbf{x}'(t), \mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \boldsymbol{\theta}, t) = \mathbf{0}$$

$$\mathbf{g}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \boldsymbol{\theta}, t) = \mathbf{0}$$

$$\mathbf{h}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \boldsymbol{\theta}, t) \leq \mathbf{0}$$

$$\mathbf{x}(\mathbf{0}) = \mathbf{x}_0$$

→ **Plugins, Reformulations, Transformations**

OCFE, Backward Euler, MPC, initialization, 2-tiered, Homotopy, Shutdown, MPEC constructs

…many different output forms.

- **MATLAB / INTLAB AD**
- **gPROMS**
- **Maple**
- **AMPL** →
  - **Optimization Solvers**: IPOPT, CONOPT, Bonmin, CPLEX, etc.
  - **Reporting/Visualization**: JSON, HTML/Sparklines, MATLAB, Matplotlib
- **LaTeX**
- **DAEOC: Fortran/C++**

Remarks

- **Challenges**
  - Trajectory profile initialization.
  - Numerical issues, scaling, solution nonuniqueness.

Typical Problem Stats	
DAE:	29 differential, 336 algebraic
NLP:	35,352 variables, 38,985 constraints, 103,282 Jacobian nonzeros.
Sol. time:	352 secs (two-tiered).

- **Current & Future work**
  - Model discontinuities: induced shutdowns, minimum shutdown duration.
  - Optimal plant specification relaxation during partial shutdown.
  - MILP-based multiple linear models for unit startups/shutdowns:
    - Partitioning of nonlinear space.
    - Incorporation of event/sequencing logic.
    - Disjunctive formulations, convex hull relaxations.
  - Closed-loop studies.

Dynamic Optimization of Electric Arc Furnace (EAF) Operation

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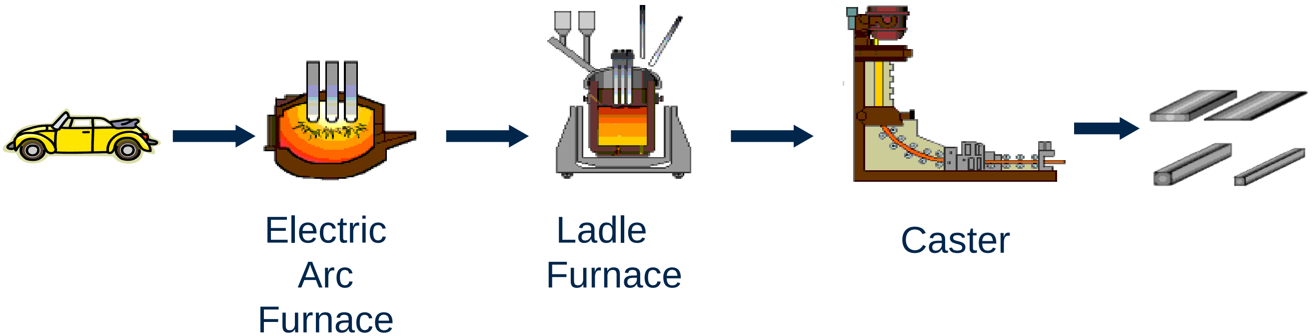


Background & Motivation

- EAF operation accounts for 40% of steel production in North America.
- Highly energy-intensive process
- Motivates development and implementation of optimization-based strategies for operation and control

Goal

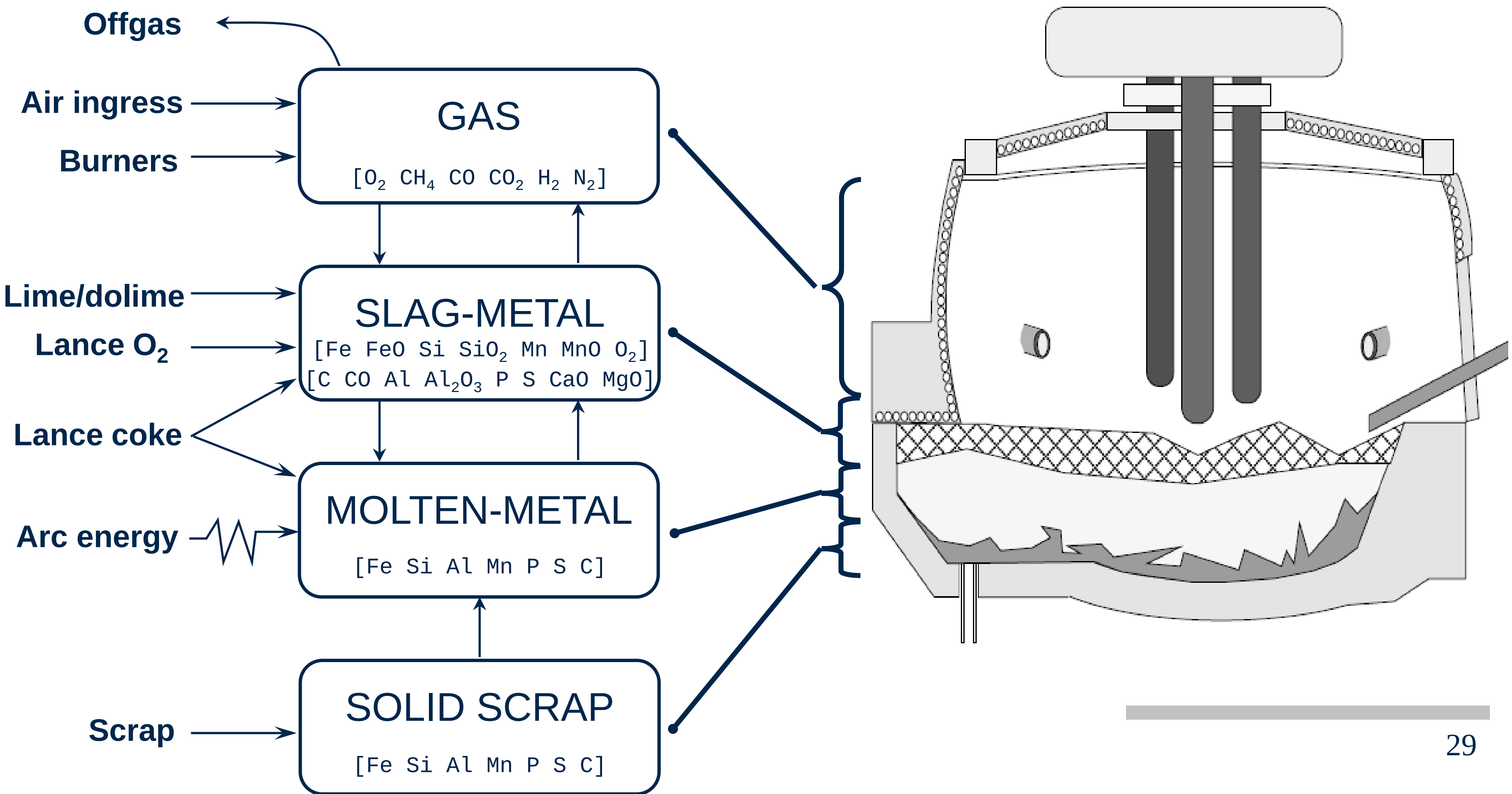
To develop a decision-support tool to determine economically optimal policies for EAF operation subject to prevailing constraints.

- Development and validation of dynamic model.
- Optimal control calculation.
- Feedback correction.

Collaboration with ArcelorMittal Dofasco

Modeling Approach

- Multi-zone System
  - Chemical equilibrium within zones
  - Reaction limited by mass transfer
- Based on mass and energy balances with equilibrium, diffusion and heat transfer relationships, and includes effects of slag foaming



Model Details

Material

- Element balances

$$\frac{d}{dt}\left(b_{k,z}\right) = F_{k,z}^{in} - F_{k,z}^{out}$$

- Equilibrium

$$\sum_i n_i a_{ik} = b_k$$

$$\Delta G_{f,i}^{o} + RT\ln(\hat{a}_i) + \sum_k \lambda_k a_{ik} = 0$$

- Net flow into zone includes
  - external flows
  - inter-zone transfer driven by concentration gradients

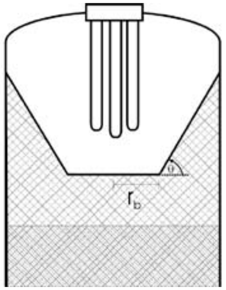
Formulated as DAE system within gPROMS; 85 differential and 1050 algebraic variables.

Energy

$$\frac{d}{dt}(E_z) = Q_z + \sum_{i=1}^{n} F_{i,z}H_{i,z}\Big|_{in} - \sum_{i=1}^{n} F_{i,z}H_{i,z}\Big|_{out}$$

$$E_z = \sum_{i=1}^{n} n_{i,z}H_{i,z}$$

- Heat flow Q_z includes
  - direct energy input
  - energy transfer by radiation
  - convective heat transfer



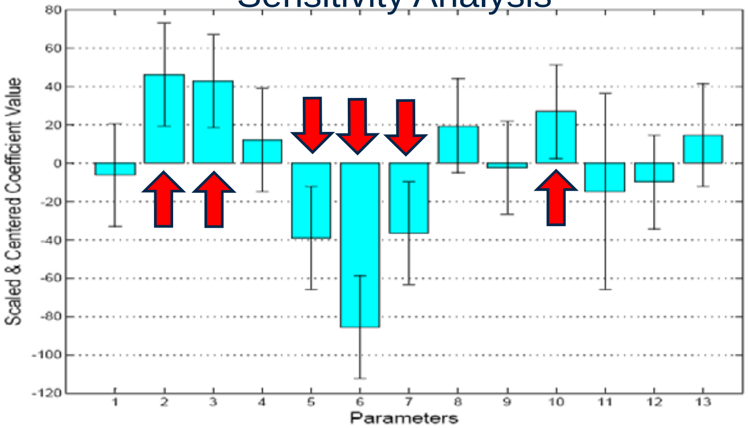
Additional Model Features

- Radiative heat transfer
- Scrap melting
- Insulating effect of slag foaming
- Variable scaling and smoothing of derivative discontinuities

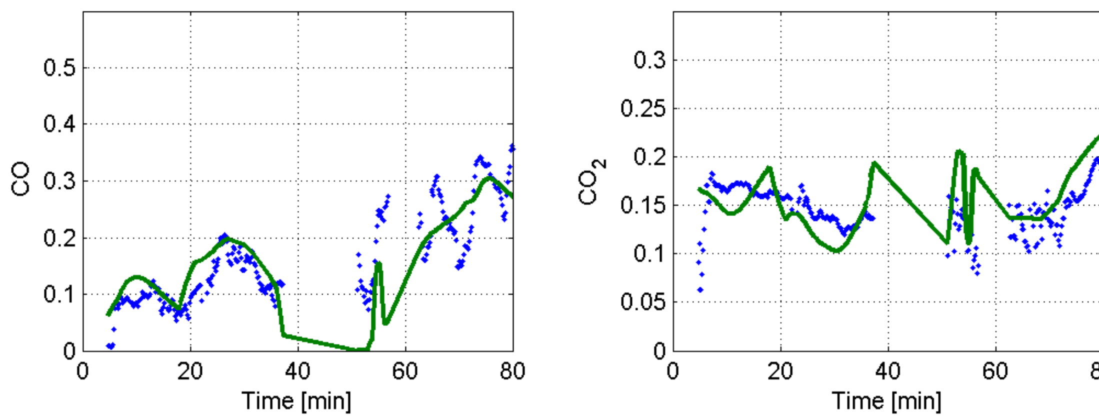
Parameter Estimation

- Sensitivity analysis to identify parameters for rigorous estimation. Based on
  - orthogonal design of experiments on parameters
  - linear regression analysis.
- Maximum-likelihood estimation via gPROMS/gEST.
- 6 parameters estimated using data from 8 EAF batches.
- Model validated against two additional data sets.

Sensitivity Analysis



Offgas Chemistry Prediction



Optimization Formulation

$$\max_{\mathbf{u}(t)} Z_{O-1} = c_0 M_{steel}(t_f) - \left(c_1 \int_0^{t_f} P dt + c_2 \int_0^{t_f} (F_{O_2,brnr} + F_{O_2,lnc}) dt + c_3 \int_0^{t_f} F_{CH_4,brnr} dt \right.$$
$$\left. + c_4 \int_0^{t_f} F_{C,inj} dt + c_5 \int_0^{t_f} F_{C,chg} dt + c_6 \int_0^{t_f} F_{flux} dt + c_7 \int_0^{t_f} F_{scrap} dt \right)$$

Model equations:

$$\mathbf{0} = \mathbf{h}\left(\dot{\mathbf{x}}(t), \mathbf{x}(t), \mathbf{u}(t), \mathbf{y}(t), t\right)$$

Input constraints:

$$P_i^{min}(t) \le P_i \le P_i^{max}(t)$$
$$F_i^{min}(t) \le F_i \le F_i^{max}(t)$$

Endpoint constraints:

$$m_{solid}(t_f) \le \epsilon$$
$$y_{\mathrm{C}}(t_f) \le Y_c^{max}$$

Path constraints:

$$T_{wall} \le T^{max}$$
$$V_{steel} \le V_{furnace}$$

P	$=$	electrical power
$F_{O_2,brnr}$	$=$	burner O_2
$F_{O_2,lnc}$	$=$	lance O_2
$F_{CH_4,brnr}$	$=$	burner CH_4
$F_{C,inj}$	$=$	injected C
$F_{C,chg}$	$=$	charged C
F_{flux}	$=$	lime/dolime

Case 1 – Base vs Optimal

Case 1 - Base vs Optimal

- Timing of second scrap charge, and initiation of carbon injection and lancing constrained to coincide with base case.
- Base case power input trajectory used as upper bound for optimal case.

Result

1. Optimal solution improves profit of heat by 8.4%
2. Burners operate at full capacity for longer period, allowing larger second scrap charge.
3. Less CO in off-gas – CO combusted in preference to CH_4 resulting in
   - cost saving due to lower CH_4 usage
   - cleaner and smaller volume of off-gas

Case 2 – Electrical Cost

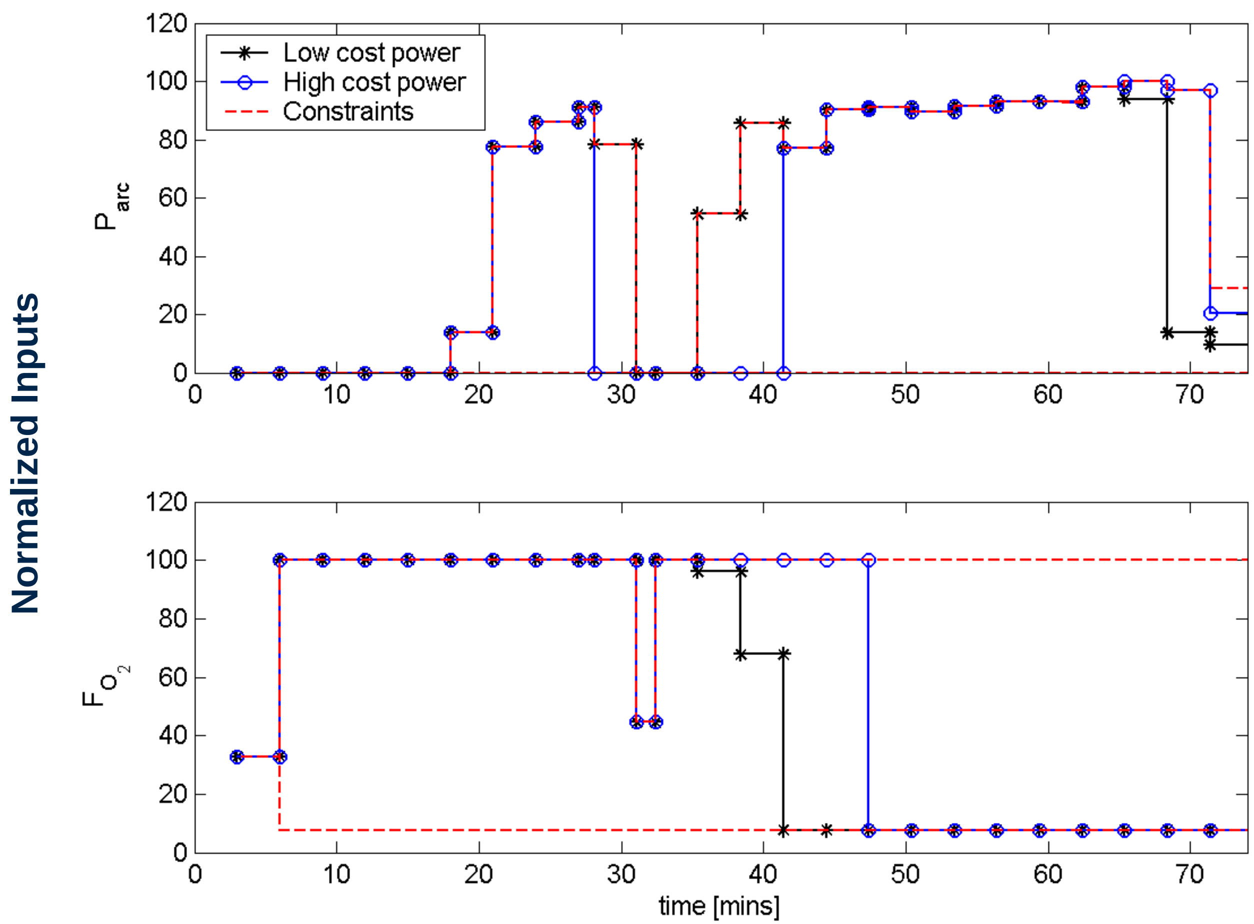
Scenarios compared

- A: Optimization at electricity cost of $0.03/kWh
- B: Optimization at electricity cost of $0.28/kWh

Result

- Scenario B compared to A gives:
  - lower power consumption
  - introduction of a second pre-heat

Input Profiles - Case 2



Remarks

- Solution time and robustness not suitable for industrial implementation.

- Demonstrates potential benefits of optimization and provides benchmark for reduced-order approaches

- Current and future work:
  - Reduced-order models
    - Reduction of model complexity
    - Data-driven models
  - State and parameter estimation for real-time implementation
  - Robust and efficient solution approaches

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