# Boundary Management of a Thermal Oxidizer

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# Outline

- Overview of Advanced Process Monitoring (APM)
- Boundary Management of a Thermal Oxidizer
  - Safety Constraints
  - Environmental Constraints
  - Economic Considerations
- Design Optimization
- Dynamic Modeling
- Keeping the Process Within Bounds

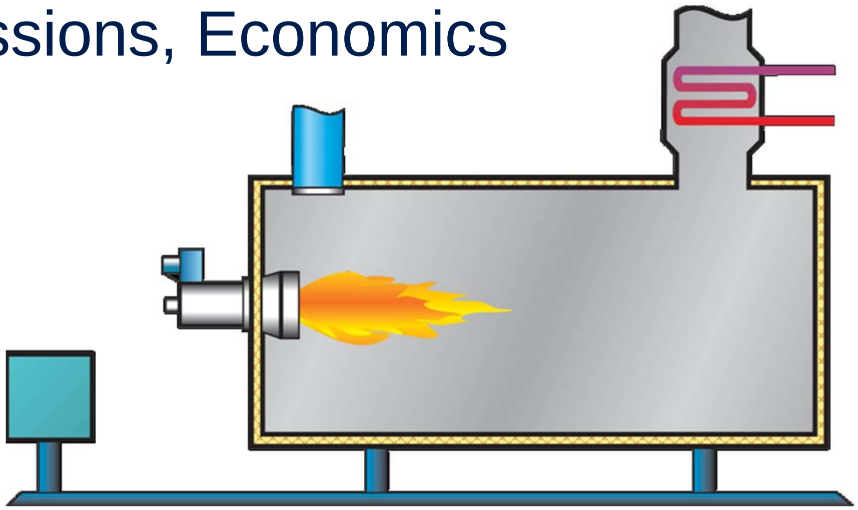
# Boundaries Are Dynamic

- Boundaries influenced by:
  - Changing economics
  - Changing feedstocks
  - Fouling, plugging (largest loss source in Petrochemicals)
  - Changing regulations

- Levels of Boundaries
  - Equipment Design Limitations / Safety Limits
  - Environmental / Emissions
  - Process Operating Window (POW)
  - Economics / Profitability

# Thermal Oxidizer Case Study

- Control emissions of volatile organic compounds (VOC)
- Industries Employing RTOs
  - Refineries
  - Petrochemicals
  - Coal Industry
  - Primary Metal Industries
  - Stone, Clay, and Glass production
- Boundaries for Safety, Emissions, Economics



# Environmental Constraints

- EPA standards
  - Highest allowable VOC composition in exiting waste gases
- Boundary Management Challenge
  - Predict the lowest required fuel amount to the burner to achieve desirable VOC Concentration in the outlet gas

# Economic Constraints

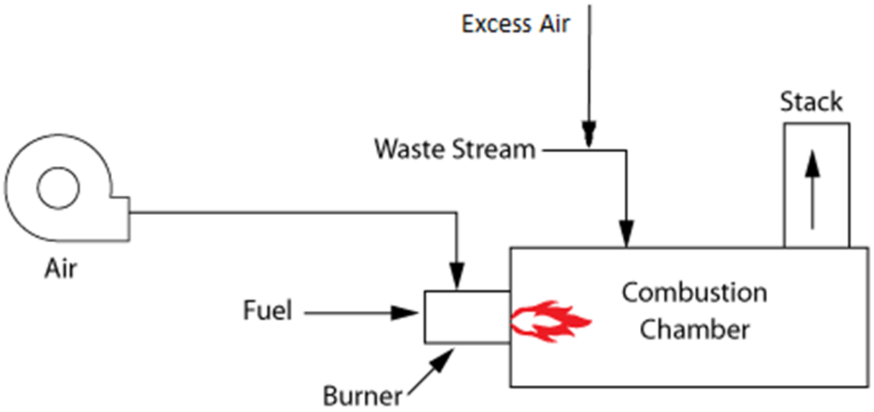
- Manipulated Variables
  - Waste gas inlet flow rate
  - Additional air to mix with waste gas
  - Burner Fuel Flow Rate
  - Burner Air Flow Rate
- Minimize Operating Costs (Natural Gas)
- Minimize Capital Costs (Size, Insulation)

# Safety Constraints

- LEL (lower Explosion Limit)
  - Inlet gas composition < 25% of LEL
- Minimum oxygen concentration
- Flashback Velocity
  - Inlet gas velocity > minimum safety limit
- Failure to observe safety constraints may lead to deflagration of waste gases back to operating units

# Design Objectives

- Control CO and O2 (>3%) exit concentrations
- Adjusting fuel and excess air
- Design Considerations
  - Temperature
  - Residence time
  - Inlet concentrations
  - Insulation costs
  - Mixing!



# Equations Used for Modeling

- Component Material Balances (each Species)
- Total Material Balance
- Reaction Rates
- Energy Balance
- Pressure Equation

# Component Material Balances

**Change of moles per time = inlet molar flow rate –outlet molar flow rate – disappearance**

- y_CO[1:Ns] * $n[1:Ns] + n[1:Ns] * $y_CO[1:Ns] = y_CO[0:Ns-1] * Ff[0:Ns-1] - y_CO[1:Ns] * Ff[1:Ns] + r_CO[1:Ns] * V[1:Ns]
- y_O2[1:Ns] * $n[1:Ns] + n[1:Ns] * $y_O2[1:Ns] = y_O2[0:Ns-1] * Ff[0:Ns-1] - y_O2[1:Ns] * Ff[1:Ns] + r_O2[1:Ns] * V[1:Ns]
- y_CO2[1:Ns] * $n[1:Ns] + n[1:Ns] * $y_CO2[1:Ns] = y_CO2[0:Ns-1] * Ff[0:Ns-1] - y_CO2[1:Ns] * Ff[1:Ns] + r_CO2[1:Ns] * V[1:Ns]
- y_H2O[1:Ns] * $n[1:Ns] + n[1:Ns] * $y_H2O[1:Ns] = y_H2O[0:Ns-1] * Ff[0:Ns-1] - y_H2O[1:Ns] * Ff[1:Ns]
- 1 = y_CO[1:Ns] + y_O2[1:Ns] + y_CO2[1:Ns] + y_N2[1:Ns]+y_H2O[1:Ns]

# Additional Equations

## Total Material Balance

**Change of moles per time = inlet molar flow rate –outlet molar flow rate – disappearance**

- $n[1:Ns] =Ff[0:Ns-1] - Ff[1:Ns] + 1/2 * r_CO[1:Ns] * V[1:Ns]

## Energy Balance

**Change of Enthalpy per time = inlet Enthalpy Flow Rate–outlet Enthalpy flow rate + Heat Generated by reactions + Heat generated by Burner**

- (Cp*(T[1:Ns]-298)*$n[1:Ns]+ Cp*n[1:Ns]*$T[1:Ns]) = Ff[0:Ns-1] * Cp * (T[0:Ns-1]-298) - Ff[1:Ns] * Cp *(T[1:Ns]-298) + (Q_rxn[1:Ns]) +Q_burner[1]

## Pressure Equation

P[1:Ns]* V[1:Ns] = n[1:Ns] * R * T[1:Ns]

# Reaction Rates

$$R_{CO} = A exp\left(\frac{-E}{RT}\right)[CO][O_2]^{0.5}[H_2O]^{0.5}$$

- r_CO[1:Ns]  = - y_CO[1:Ns] * y_O2[1:Ns]^0.5*y_H2O[1:Ns]^0.5 *exp(-E/(1.987*T[1:Ns]))*k0*(P[1:Ns]/(82.06*T[1:Ns]))^2

r_CO2[1:Ns] =  -  r_CO[1:Ns]

r_O2[1:Ns]  =  0.5 * r_CO[1:Ns]

# Optimizing the Design

- ## Design Decisions

| |
|---|
| Volume of Thermal Oxidizer (m^3) |
| Fuel Flow Rate (m^3/h) |
| Air Flow Rate (mol/s) |

- ## Objective – Minimize Cost

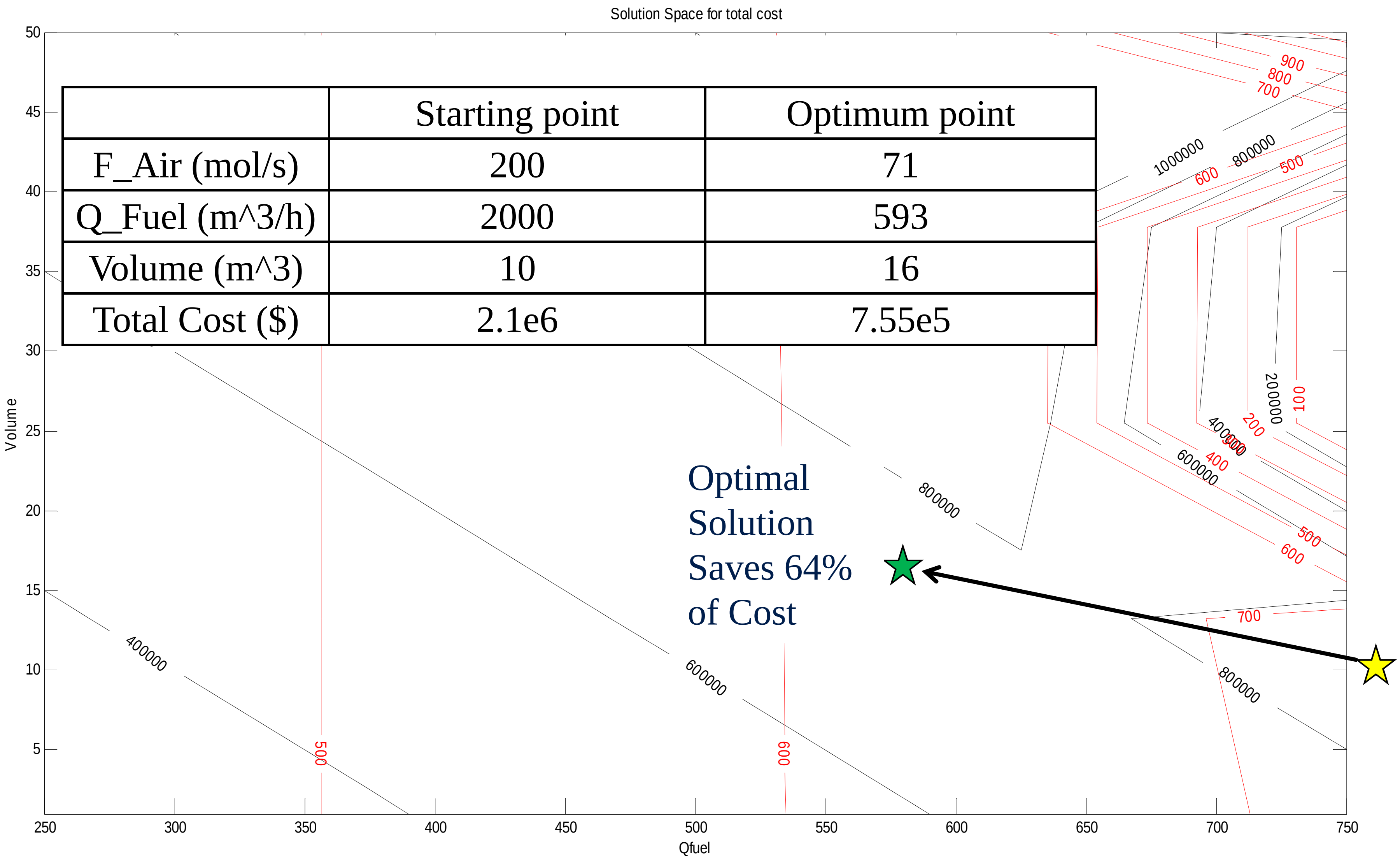
| |
|---|
| Total Cost = (Insulation and Construction Cost per Volume) * Volume + (Burner and Operating Cost per Fuel Flow Rate) * Fuel Flow Rate |

- ## Constraints

| |
|---|
| Minimum Oxygen Outlet Concentration = 3% |
| Minimum CO outlet Concentration = 1% |

# Starting Point vs. Optimal Design

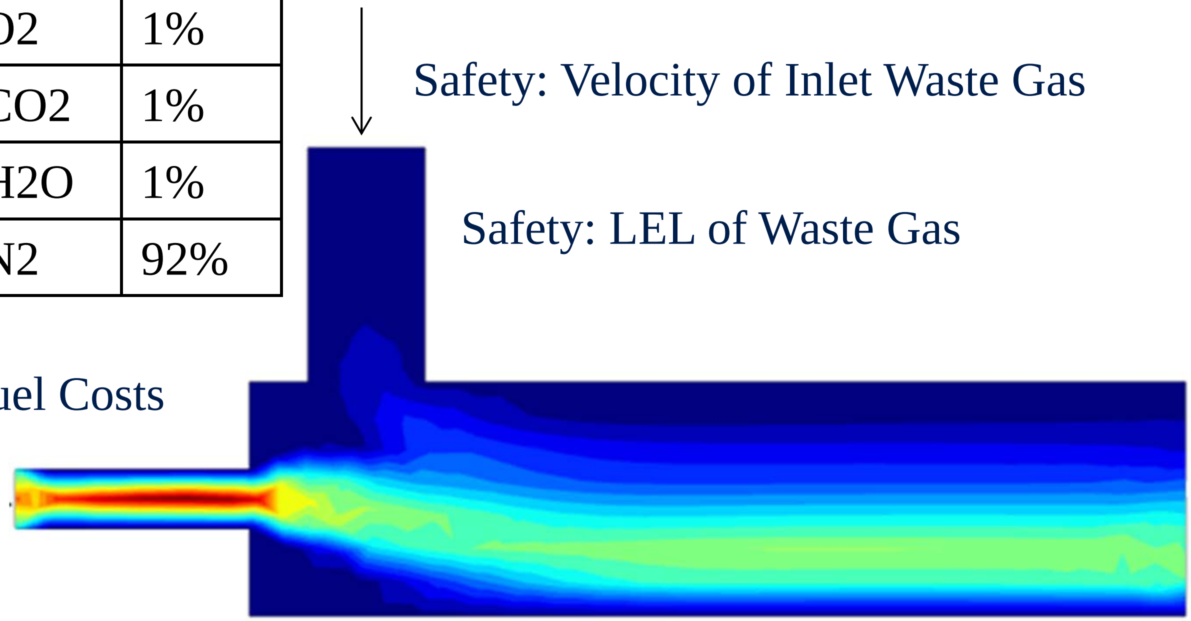
| | Starting point | Optimum point |
|---|---|---|
| F_Air (mol/s) | 200 | 71 |
| Q_Fuel (m^3/h) | 2000 | 593 |
| Volume (m^3) | 10 | 16 |
| Total Cost ($) | 2.1e6 | 7.55e5 |



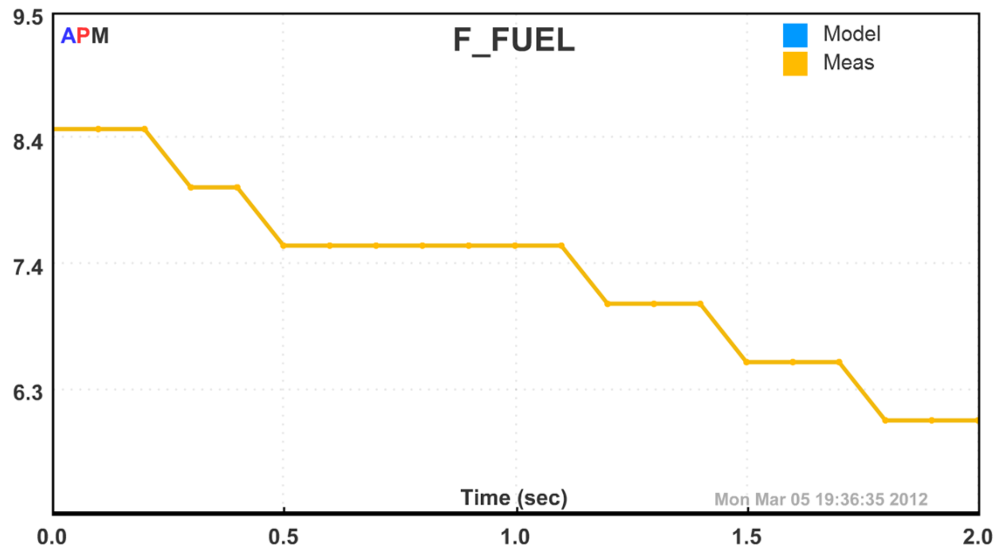
# Modeling Dynamic Boundaries

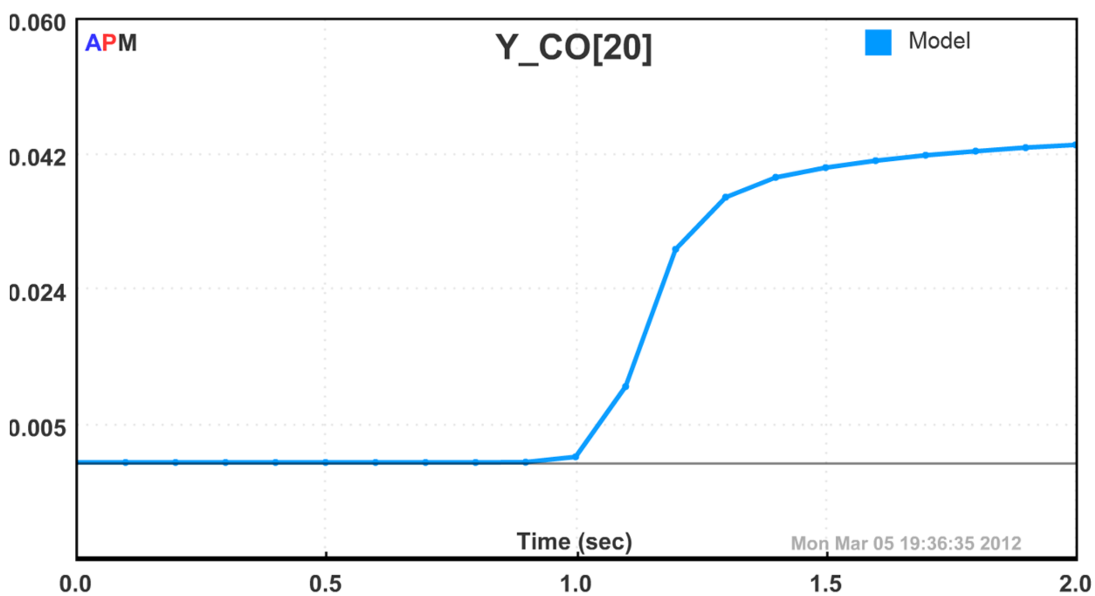
- Model predicts boundary values for safe, responsible, and economic operating conditions

| | |
|---|---|
| CO | 5% |
| O2 | 1% |
| CO2 | 1% |
| H2O | 1% |
| N2 | 92% |

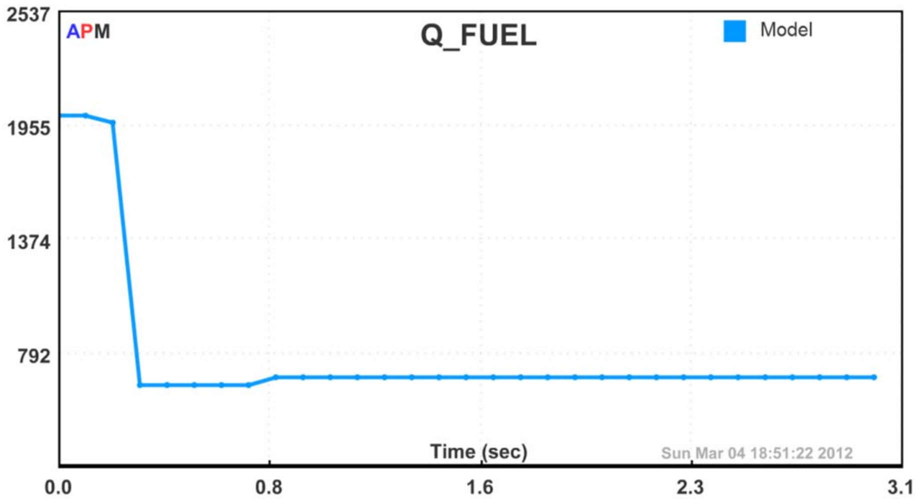


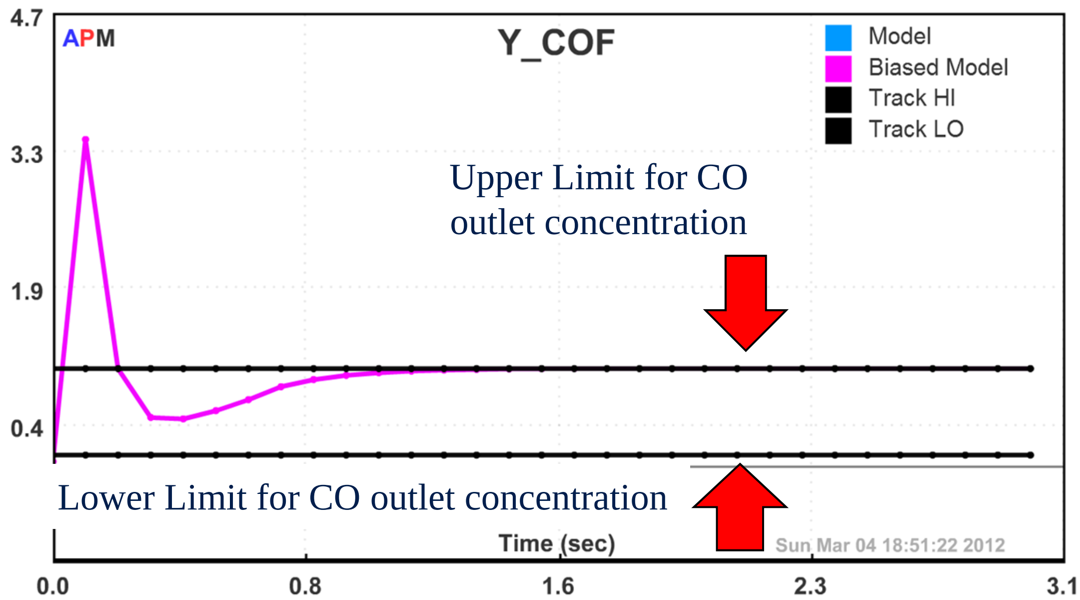
# Dynamic Modeling Results



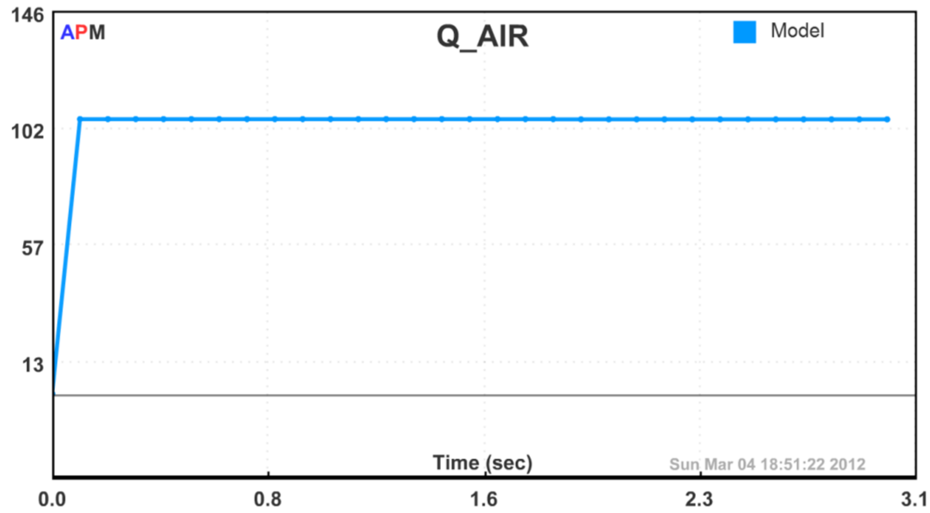



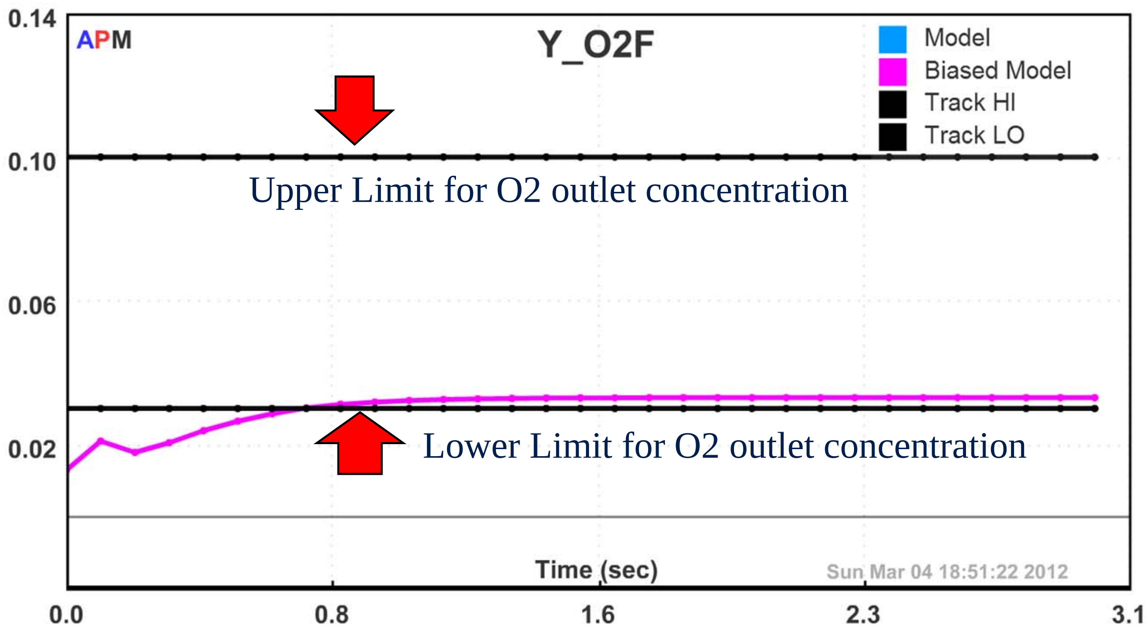
# Maintain Bounds for CO Concentration



# Maintain Bounds for O2 Conc



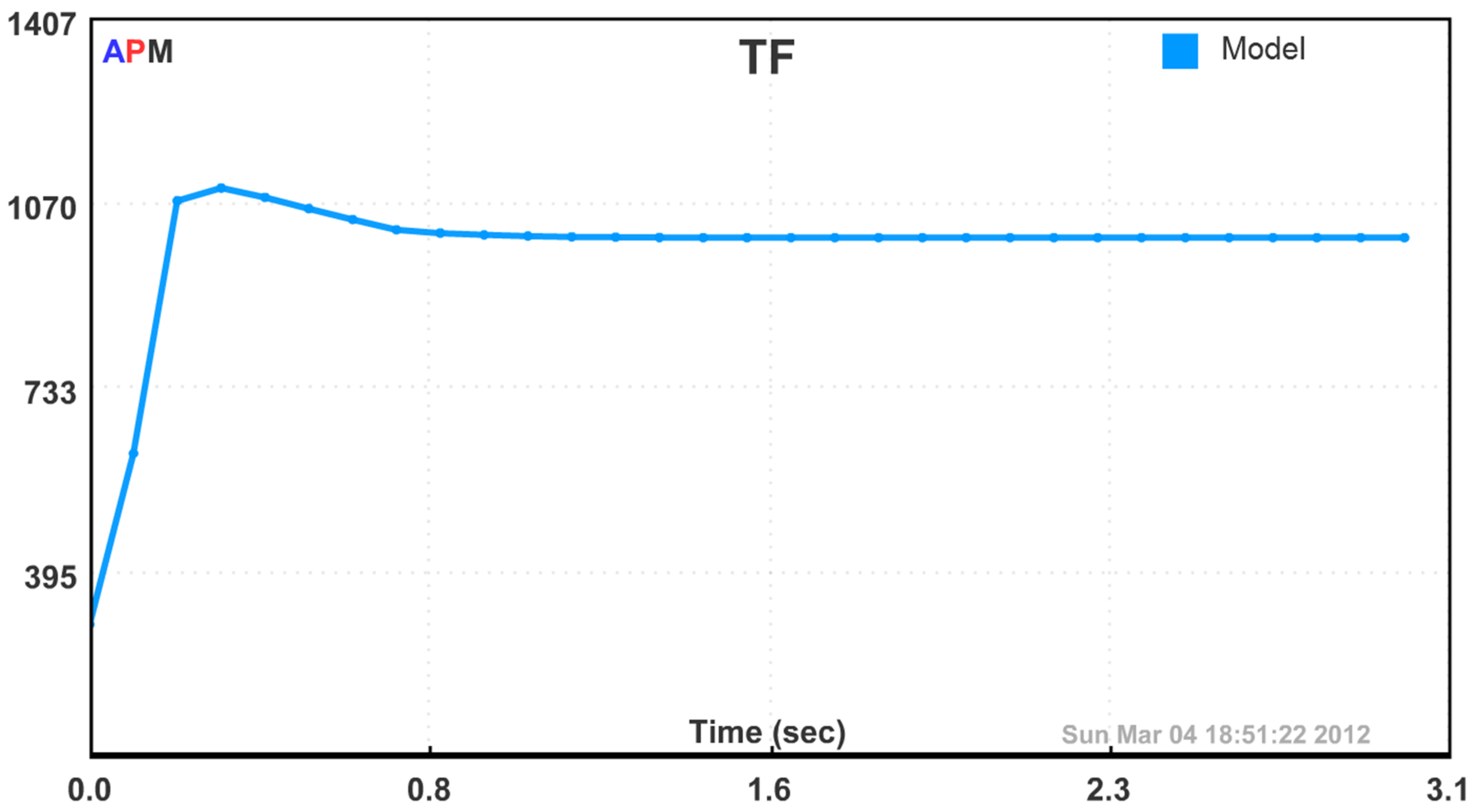



# Summary

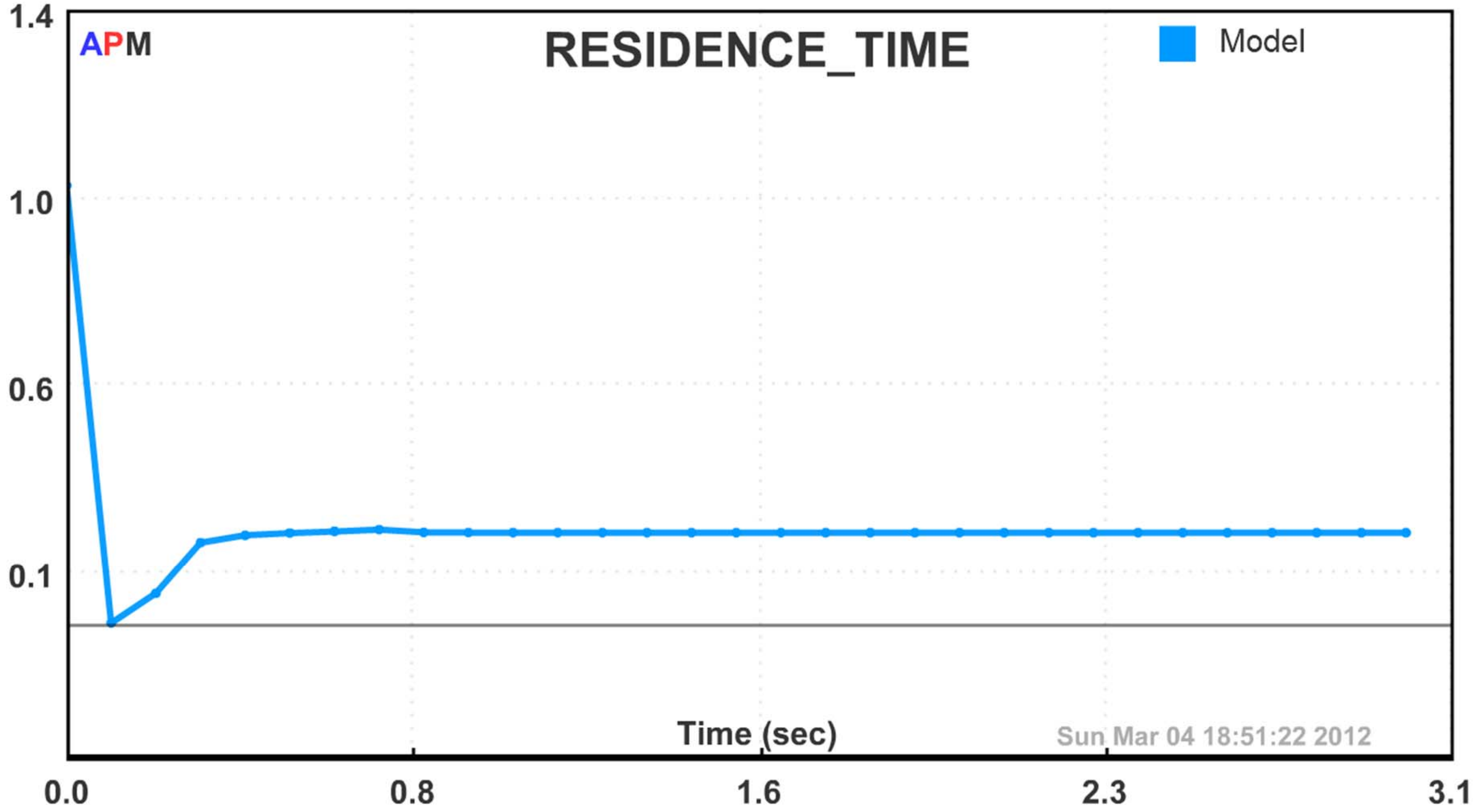
- Boundary Management
  - Static Constraints
  - Dynamic Constraints
- Model-based Boundary Management
  - Empirical (Fast) or First Principles (Accurate) Models
  - Monitor Safety, Environmental, and Economic Constraints
- Thermal Oxidizer Case Study as a Demonstration

# Additional Slides

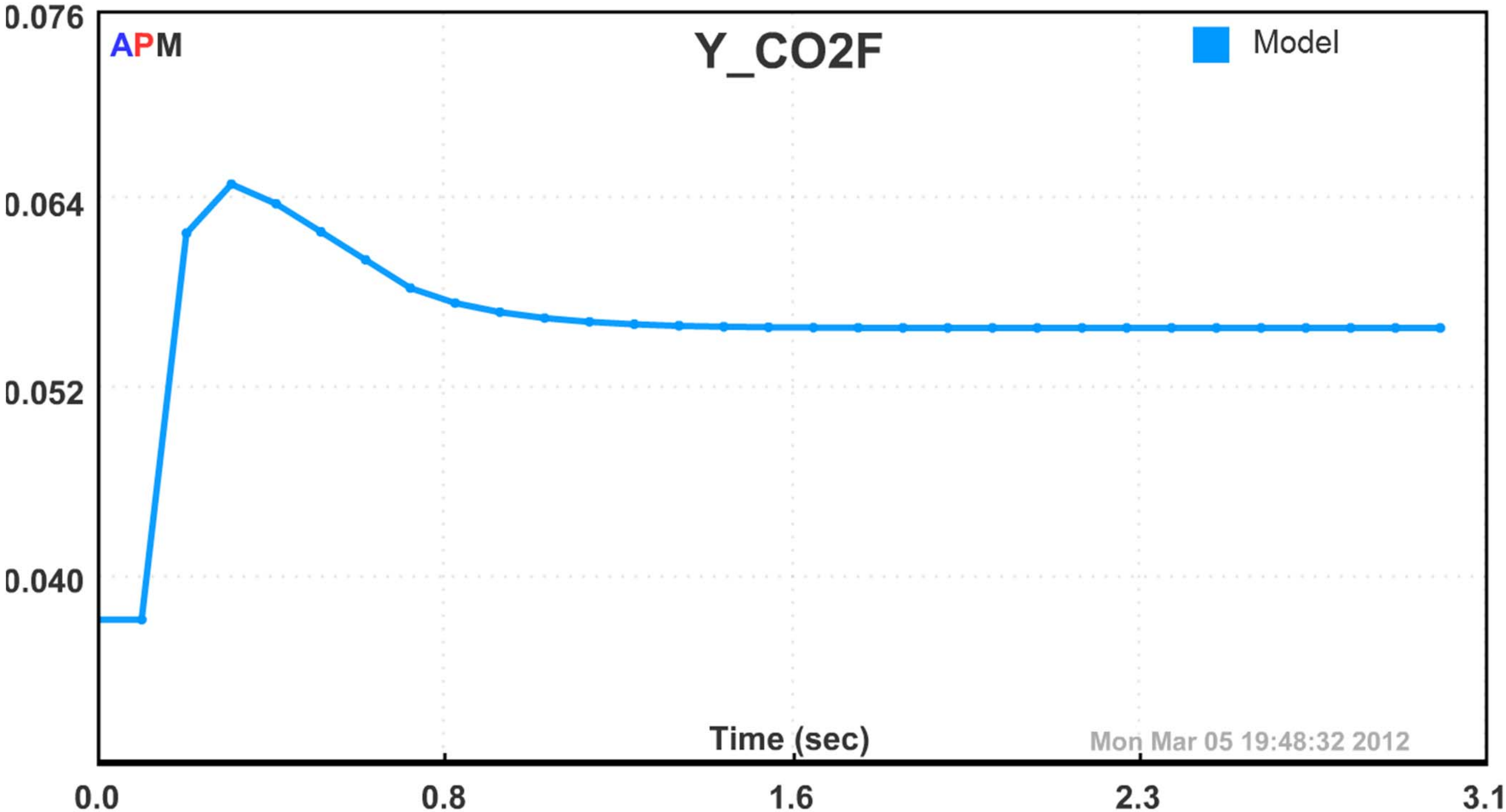
# Temperature Change



# Residence Time Change



# Carbon Monoxide Concentration Change



# H2O Concentration Change