DYNAMIC MODELING
FUEL PROCESSORS

PROJECT GOALS

- Develop detailed dynamic models of fuel processor (FEMLAB) and fuel cell components (Simulink) for aeronautical applications
- Integrate models into a common framework for dynamic simulation and analysis using Simulink
- Evaluate and refine approach for reusability, rapid development and assessment of complete system, and design improvement from simulation results

BACKGROUND

- Fuel cell based power systems are becoming increasingly important in aeronautical applications
- Reformer based fuel cell systems make the technology amenable to logistic fuels such as diesel, JP5 and JP8
- A fundamental analysis of the dynamic system response is a critical factor in the overall design process.
- Detailed dynamic models of the fuel reformer – fuel cell system will become a key tool for carrying out design analyses.

Dynamic Simulation Approach

Modular Approach:

Individual simulation modules for each fuel cell type

- Tubular SOFC
- Planar SOFC
- MCFC
- PEM

Reformer module

Gas turbine module (compressor and turbine sub-modules)

Catalytic oxidizer Combustor module

Heat exchanger module

Humidifier module

Condenser module

Pumps, valves, regulators, plumbing, and other balance of plant (BOP)

Standardized Framework For Dynamic Modeling & Controls

- Collaboration between Control group (Prof. F. Jabbari) and Dynamic Simulation (Prof. S. Samuelsen, J. Brouwer, …)
- MATLAB and SimulinkTM Framework Chosen
- User friendly package by MathWorks (Matlab)
- Flexibility
    - Prepackaged modules
    - Object oriented
    - Easy to learn and use
    - Hardware extensible
    - Transferable to other software
- Natural for adding controls development and power electronics

Previous Module Development
Reformer, SOFC, MCFC, PEM, Gas Turbine

General Model Assumptions

- 1D process flow
- Well-stirred within nodal volume
- Slow pressure transients

Fuel Cell Assumptions

- H2 electrochemically oxidized only
- CO consumed via water-gas shift
- Shift always at equilibrium (constraint)
- Equipotential: $V_{cell} = V_{node\ 1} = V_{node\ n}$

Dynamic Model Basic Equations

Equation of State

$$C = \frac{P}{R_u T}$$

Mass Conservation Equations

$$V\frac{dC_j}{dt} = \dot{N}_{in,j} - \dot{N}_j + r_j$$

$$VC\frac{d\mathbf{X}}{dt} = \dot{N}_{in}(\mathbf{X}_{in} - \mathbf{X}) - \mathbf{X}\sum r_j + \mathbf{R}$$

Calculates changes in mole fraction based on inlet molar flows and reaction rates

Dynamic Model Basic Equations

Energy Conservation

- **Gaseous**

$$\frac{d}{dt}(CC_{v,molar}T) = (\dot{N}h)_{in} - \dot{N}h + \overbrace{(\dot{N}h)_{solid\to gas}}^{\text{Molar Flow Through Electrolyte (Fuel Cell Only)}} + (\text{heat transfer}) + (\text{heat of reaction})$$

- **Solid**

$$\frac{d}{dt}(\rho C_{mass}T) = \overbrace{(\dot{N}h)_{gas1\to solid}}^{\text{Molar Flow Through Electrolyte (Fuel Cell Only)}} - (\dot{N}h)_{solid\to gas2} + (\text{heat transfer}) + (\text{heat of reaction})$$

Heat Transfer

Conduction

- Axially from node to node through solids
- Between nodal materials (bipolar plates, electrodes, …)

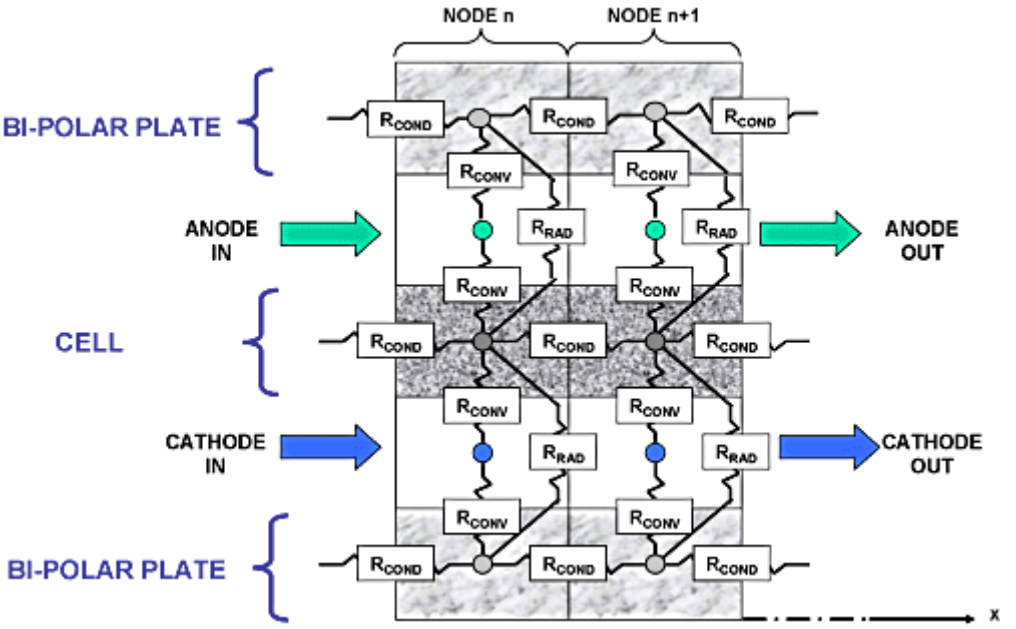
Convection

- Between surfaces and gases
- Based on Nusselt number

Radiation

- From surface to surface
- Geometry is an issue
  - Concentric cylinders: TSOFC
  - Parallel planes: PSOF
- Other: combustor, reformer

Planar Nodal SOFC Heat Transfer Resistances



Solid Oxide Fuel Cell Electrochemistry

Cell Reactions

$$H_2 + O^{2-} \xrightarrow{anode} H_2O + 2e^-$$

$$\tfrac{1}{2}O_2 + 2e^- \xrightarrow{cathode} O^{2-}$$

Nerst Potential

$$E = E_0 + \frac{R_u T}{2F} \ln\left(\frac{\chi_{H_2} \chi_{O_2}^{1/2}}{\chi_{H_2O}} P_{CATHODE}^{1/2} \right)$$

- Ideal operating voltage with respect to partial pressures of cell reactants

Steam Reformation – Occurs in Reformer and Fuel Cells

Methane reformation reaction

$$CH_4 + H_2O \xrightarrow{\text{reform}} 3H_2 + CO$$

- **Reaction rates on nickel based catalysts:** ***Lee et al. (1990) and Ross et al. (1972)***

$$r_{CH_4} = -kP_{CH_4}^m P_{H_2O}^n$$

From Stoichiometry…

$$r_{CO} = -r_{CH_4}$$

$$r_{H_2} = -3r_{CH_4}$$

$$r_{H_2O} = r_{CH_4}$$

Water Gas Shift – Occurs in Reformers and in Fuel Cells

Shift reaction

$$CO + H_2O \xleftrightarrow{\text{shift}} CO_2 + H_2$$

- **Reaction proceeds fast enough at elevated temperatures to assume equilibrium**
- **Algebraic constraint at exit of each node**

Provides the non-electrochemical reaction source for CO_2!

$$K(T) = \frac{\chi_{CO_2}\chi_{H_2}}{\chi_{CO}\chi_{H_2O}}$$

Fuel Cell Operation

Actual operating voltage

$$V = E - \eta_A - \eta_C - \eta_R$$

- **Polarization losses are due to kinetics, mass transport and electrical resistances**

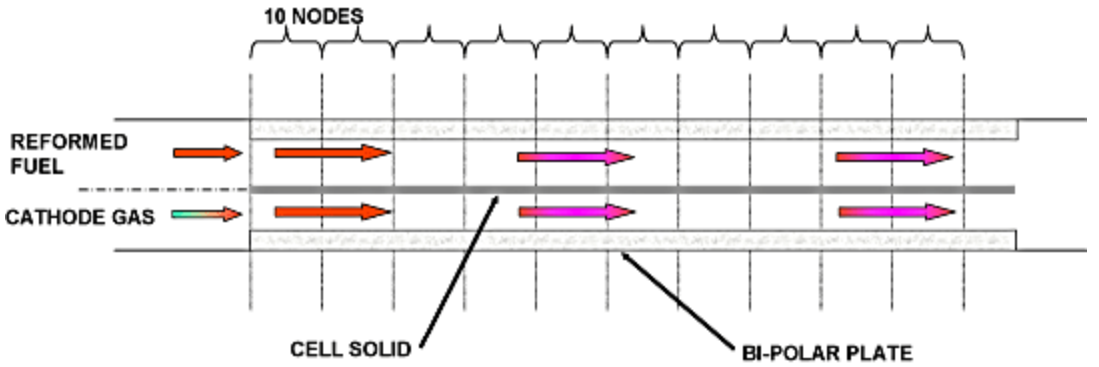
$$\eta_A = \frac{R_u T}{\alpha n F} \ln\left(\frac{i_{node}}{i_0}\right)$$

$$\eta_C = -\frac{R_u T}{nF} \ln\left(1 - \frac{i}{i_L}\right)$$

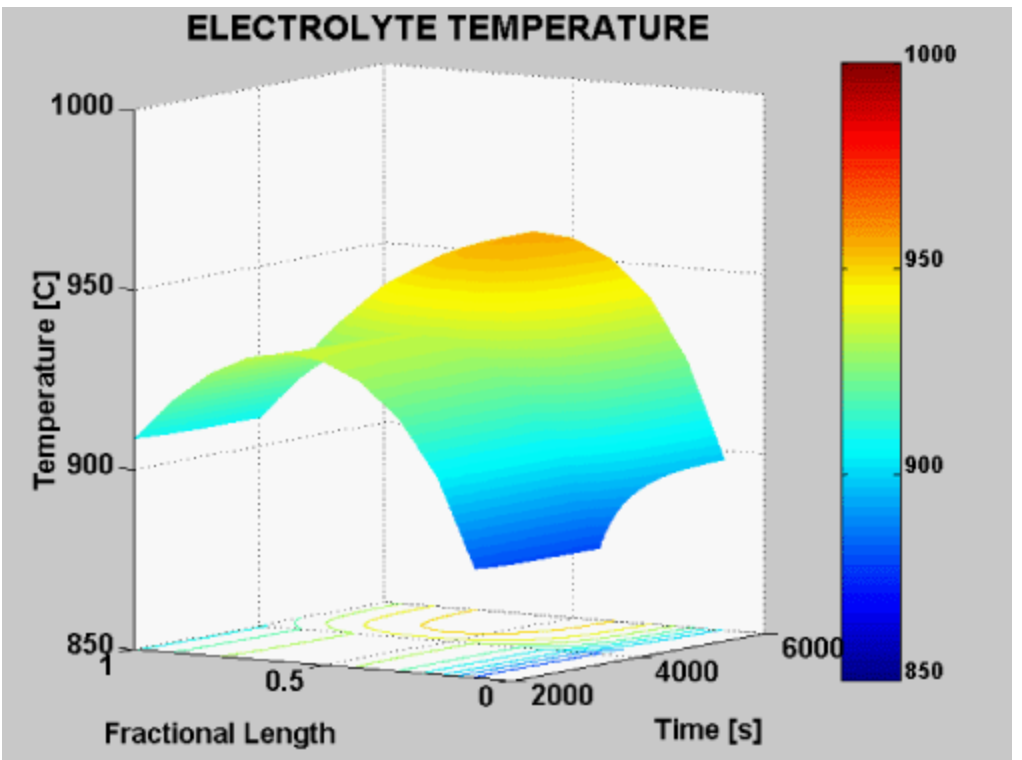
$$\eta_R = iR$$

PSOFC DISCRETIZATION

- 10 Discrete Computational Nodes
- Anode Gas
- Cathode Gas
- Cell Solid
- Bi-Polar Plate
-



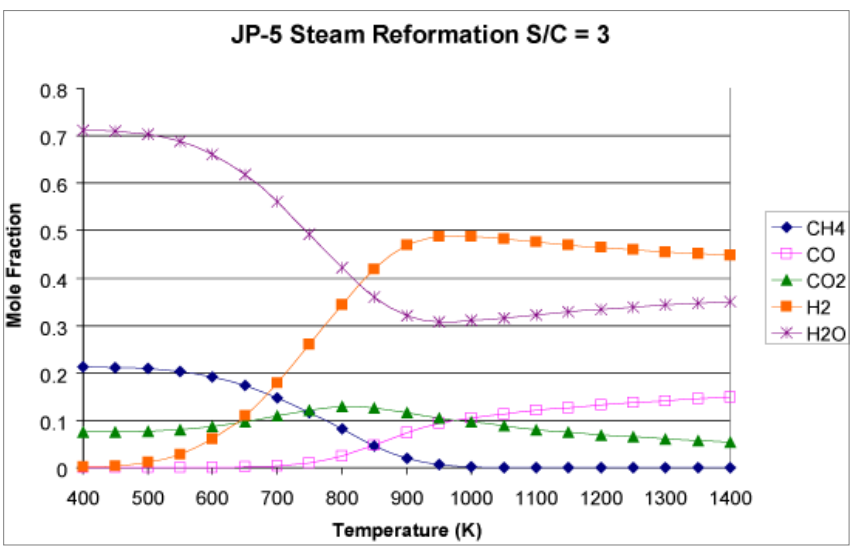
Sample TSOFC Outputs: 10% Load Increase

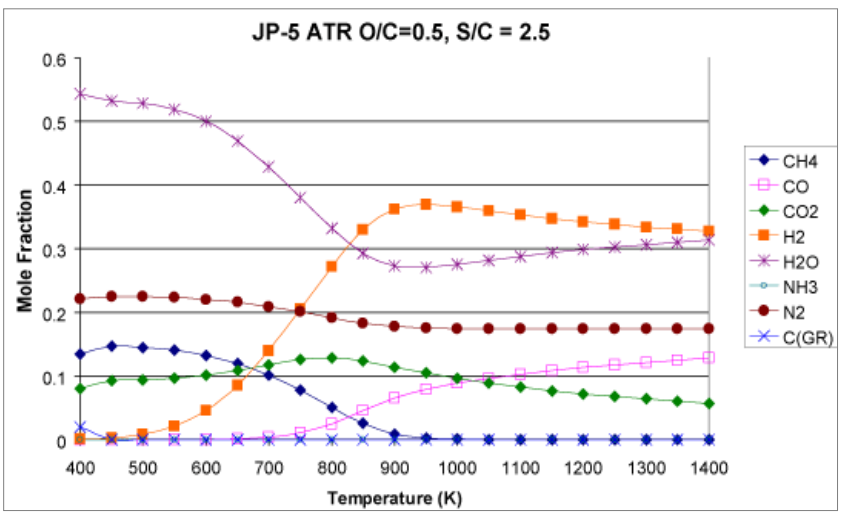


PROGRESS & CURRENT STATUS

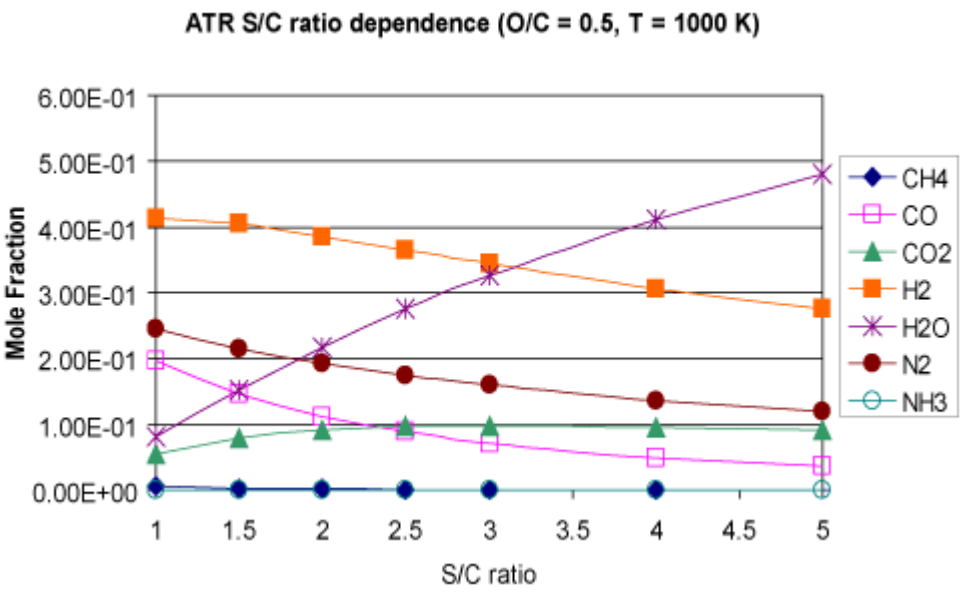
Jet Fuel Equilibrium Results

- Various Jet Fuel thermodynamic data acquired
- Commercial Aviation Fuel, Jet-A
  - C11H21
  - MW: 153 g/mol
  - Heat of formation (DHfo): -249 kJ/mol
- Traditional Air Force Military Aviation Fuel, JP-4
  - C10H19.4
  - MW: 139 g/mol
  - Heat of formation (DHfo): -227 kJ/mol
- Traditional Navy Military Aviation Fuel, JP-5
  - C10H19.2
  - MW: 139 g/mol
  - Heat of formation (DHfo): -222 kJ/mol
- Standard Military Aviation Fuel, JP-8
  - C12H23
  - MW: 167 g/mol
  - Heat of formation (DHfo): -319 kJ/mol
  -

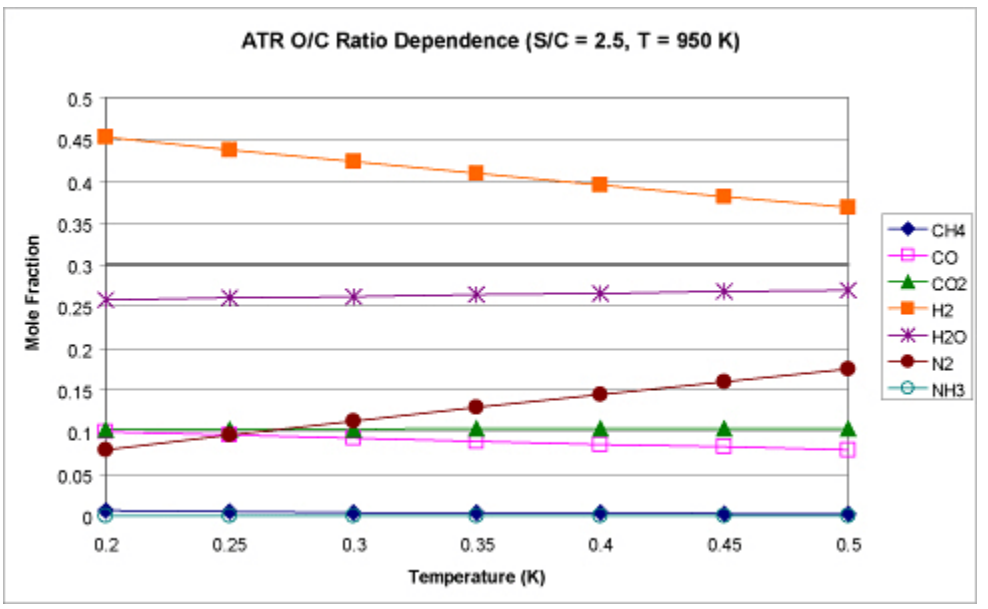




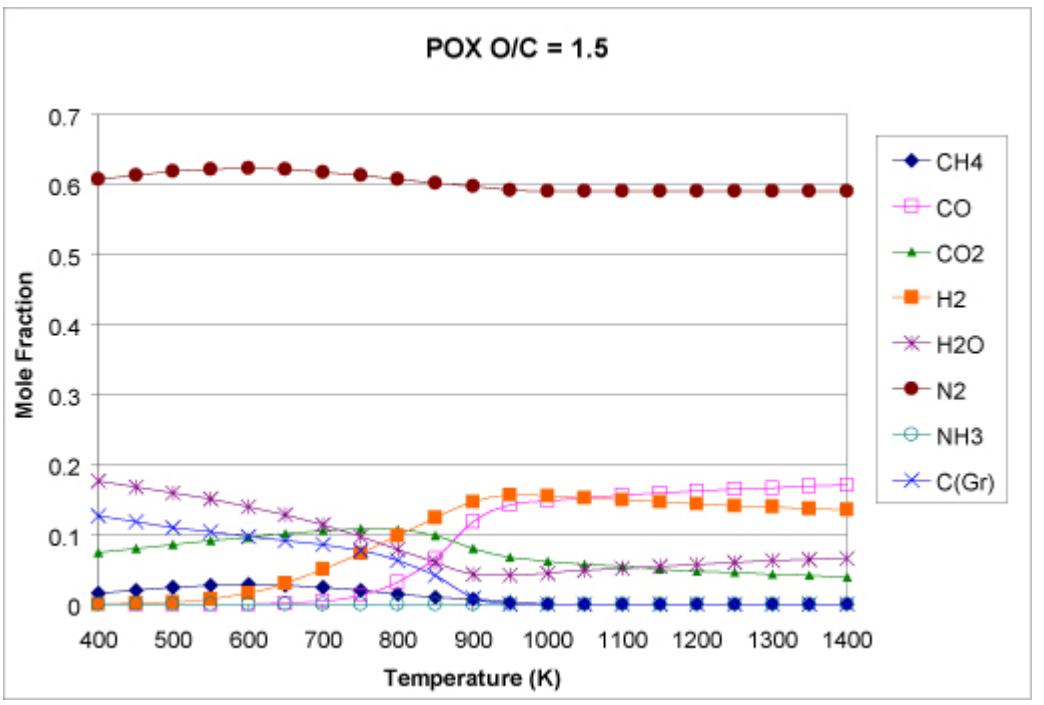
Effects of S/C



Effects of O/C



Jet Fuel Equilibrium Results – Partial Oxidation



New Module Development

•Reaction Mechanism Need and Approaches

- Use Equilibrium results in look-up tables with discretized dynamic model for heat transfer, mass and momentum conservation
- Use Chemical Kinetics from a simpler hydrocarbon set
- Obtain data and/or develop simple chemical kinetic mechanism for JP-5

•Must incorporate dynamic equations

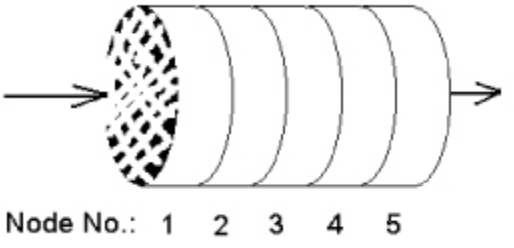
- Heat transfer (conduction, convection, radiation)
- Mass (or species) conservation
- Momentum conservation
- Energy conservation

•Main module development need is for the overall geometry of the NuElement Module

- **Dynamic JP-5 Reformer Module**
- **Concentric Cylinders**
  - Combustor
  - Catalyst Bed
  - Preheat
  - Anode off-gas recycle (option)
- **Reformation Kinetics**

- $CH_4 + H_2O = CO + 3H_2$ $\quad \Delta H^{o}_{298K} = 206\,kJ/mol \quad (1)$
- $CH_4 + 2H_2O = CO_2 + 4H_2$ $\quad \Delta H^{o}_{298K} = 165\,kJ/mol \quad (2)$
- $CH_4 + 2O_2 = CO_2 + 2H_2O$ $\quad \Delta H^{o}_{298K} = -803\,kJ/mol \quad (3)$

- **Reformer Geometry (5 nodes)**



- **Six Step Reaction Mechanism**

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2 \quad (1)$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \quad (2)$$

$$CH_4 + 2H_2O \Leftrightarrow CO_2 + 4H_2 \quad (3)$$

$$CH_4 + 2O_2 \Leftrightarrow CO_2 + 2H_2O \quad (4)$$

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2 \quad (5)$$

$$CH_4 + CO_2 \Leftrightarrow 2CO + 2H_2 \quad (6)$$

- **Arrhenius Rate Expressions**

$$k_i = A_i \exp\left(-\frac{E_i}{RT}\right)$$

$$r_1 = k_1\left(\frac{P_{CH_4}P_{H_2O}}{P_{H_2}^{2.5}} - \frac{P_{CO}P_{H_2}^{0.5}}{K_{p1}}\right)/DEN^2$$

$$r_2 = k_2\left(\frac{P_{CO}P_{H_2O}}{P_{H_2}} - \frac{P_{CO_2}}{K_{p2}}\right)/DEN^2$$

$$r_3 = k_3\left(\frac{P_{CH_4}P_{H_2O}^2}{P_{H_2}^{3.5}} - \frac{P_{CO_2}P_{H_2}^{0.5}}{K_{p3}}\right)/DEN^2$$

$$r_4 = k_4 P_{CH_4} P_{O_2}$$

$$r_5 = k_5\left(P_{CH_4}P_{H_2O} - \frac{P_{CC}P_{H_2}^3}{K_{p5}}\right)$$

$$r_6 = k_6\left(P_{CH_4}P_{CO_2} - \frac{P_{CC}^2P_{H_2}^2}{K_{p6}}\right)$$

$$DEN = 1 + K_{CO}P_{CO} + K_{H_2}P_{H_2} + K_{CH_4}P_{CH_4} + K_{H_2O}P_{H_2O}/P_{H_2}$$

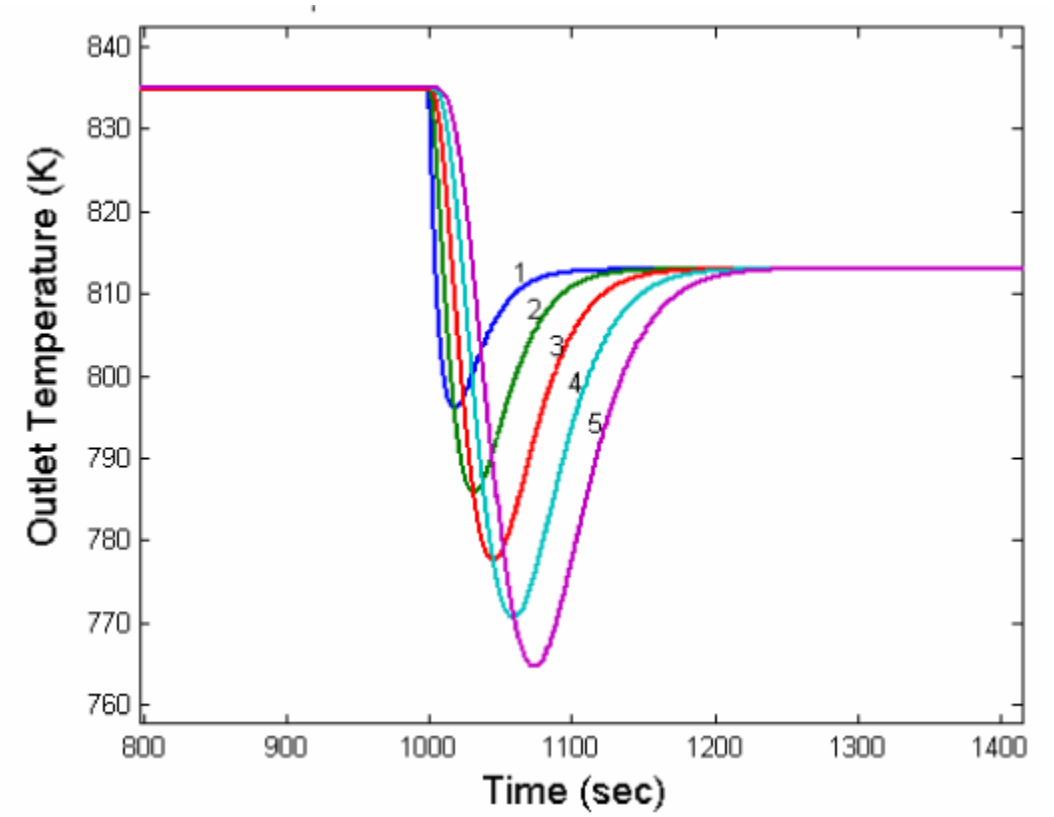
Reaction i	Activation energy E_i (kJ/mol)	Pre-exponential factor A_i
1	240.1	1.336×10^{15} (kmol*MPa$^{(0.5)}$/kg_{cat}*h)
2	67.13	1.955×10^{7} (kmol/kg_{cat}*h*MPa)
3	243.9	3.22×1014 (kmol*MPa$^{(0.5)}$/kg_{cat}*h)
4	166	1.10 (mol/g_{cat}*s*Pa^2)
5	29	4.19×10^{-9} (mol/g_{cat}*s*Pa^2)
6	23.7	2.42×10^{-9} (mol/g_{cat}*s*Pa^2)

- **Reaction Equilibrium Constants**

$$K_j = A_j \exp\left(-\frac{\Delta H_j}{RT}\right)$$

Equilibium constant K_{pi}	Dimensions
$K_{p1} = 1.198 \times 10^{11} * \exp(-26830/T)$	$(MPa)^2$
$K_{p2} = 1.77 \times 10^{-2} * \exp(4400/T)$	$(MPa)^0$
$K_{p3} = K_{p1} \cdot K_{p2}$	$((MPa)^2$
$K_{p5} = K_{p1}$	$(MPa)^2$
$K_{p6} = 6.780 \times 10^{12} * \exp(-31230/T)$	$(MPa)^2$

- **Reformer Dynamic Simulation Results – S/C 1.0 ▸ 1.5**



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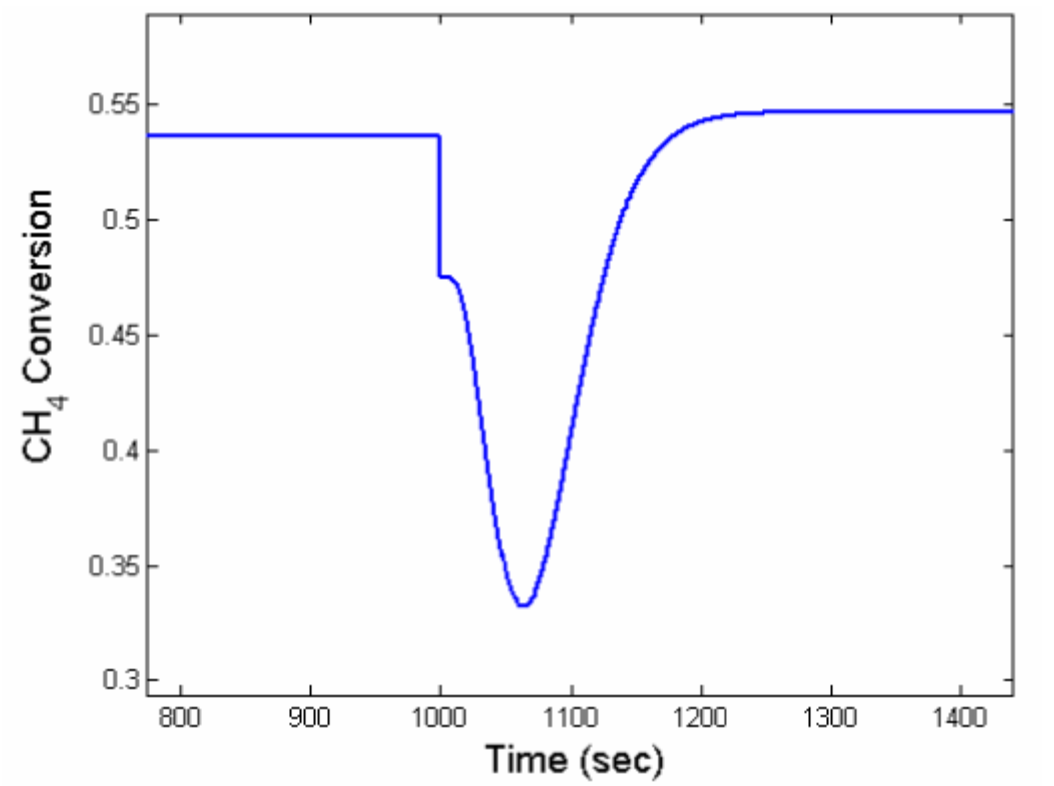
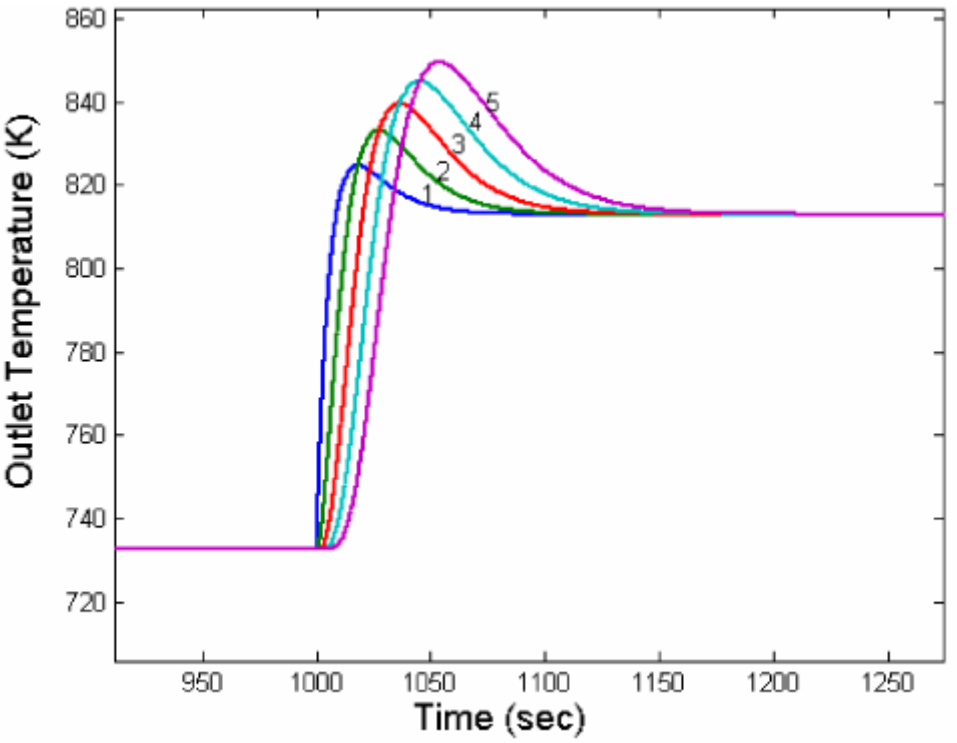
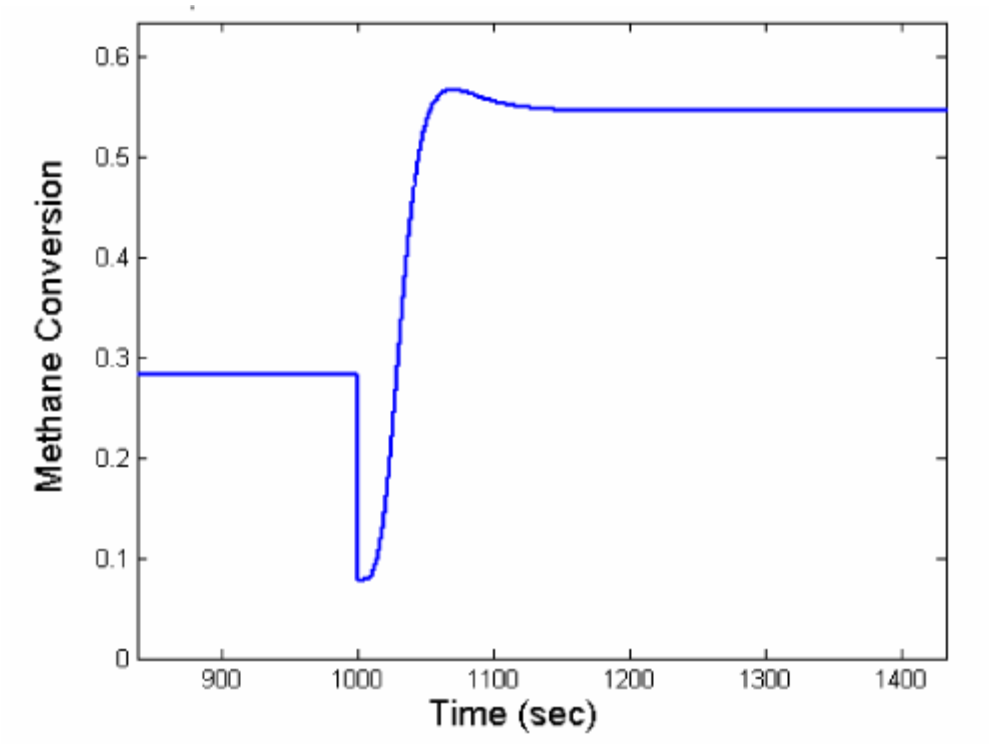


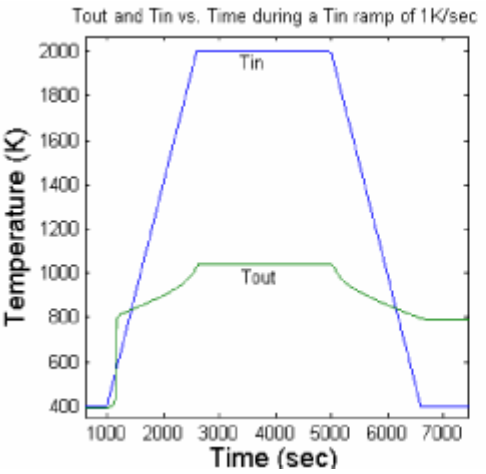
- **Reformer Dynamic Simulation Results – O/C 0.25 ▸ 0.5**

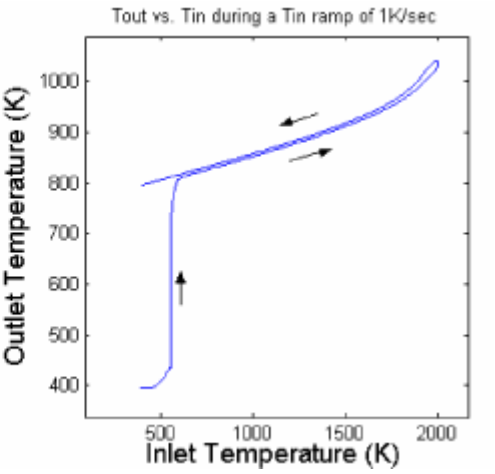


- **Reformer Dynamic Simulation Results – O/C 0.25 ▸ 0.5**



- **Reformer Dynamic Simulation Results – Catalyst “light off”**





CONCLUSIONS

- Simulink interface critical to the development of system-wide dynamic models.
- Modular approach compatible with several implementation techniques for component models, including user-written programs (FORTRAN / C) as well as commercial simulation software.

PERSONNEL

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SPONSORS

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