# 2002 PROGRAM / LAB REVIEW

## Fuel Cells for Transportation/Fuels for Fuel Cells


# Fuel Processing of Diesel for Fuel Cells

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**National Energy Technology Laboratory**

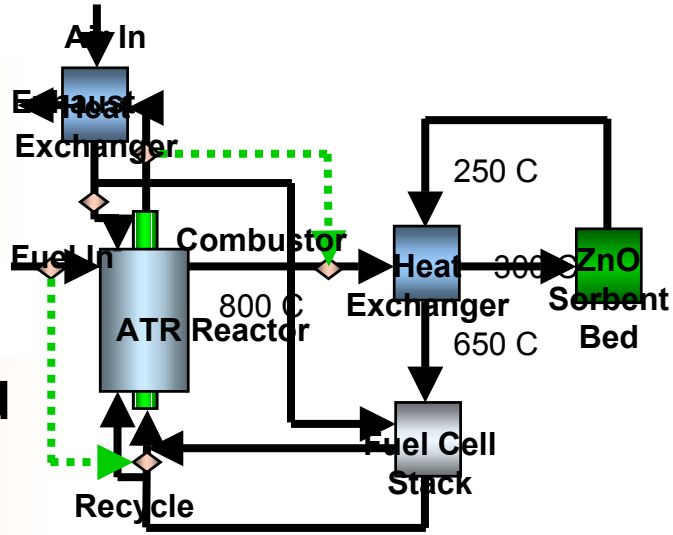
# Diesel Fuel Processing
## *Objective*

- **Objective**
  - Develop fundamental understanding of diesel fuel reforming and provide necessary tools and information to fuel cell/fuel process developers and system integrators for performance optimization and system control.
- **Technical challenges**
  - Diesel fuel is complex and difficult to reform :
    - Deactivation of fuel reforming catalysts and fuel cell components via carbon deposition and sulfur poisoning are the principle technology barriers.
    - Diesel fuel is a complex, multi-component (>100 compounds) fuel that exhibits varying reaction pathways and kinetic rates for differing catalyst types.
  - Large, complex, slow-response fuel processors problematic:
    - Several FC applications require high power density design with “fast” response and high efficiency for transient operations.
    - Hydrocarbon slip must be avoided.

# Diesel Fuel Processing

## *Technical Approach*

- **Conduct Systems Analysis to Understand Reformer Integration and Operational Requirements**




- **Utilize CFD Models to Understand and Address Heat and Mass Transfer Issues and Reactor Performance for Steady State and Transient Analysis**

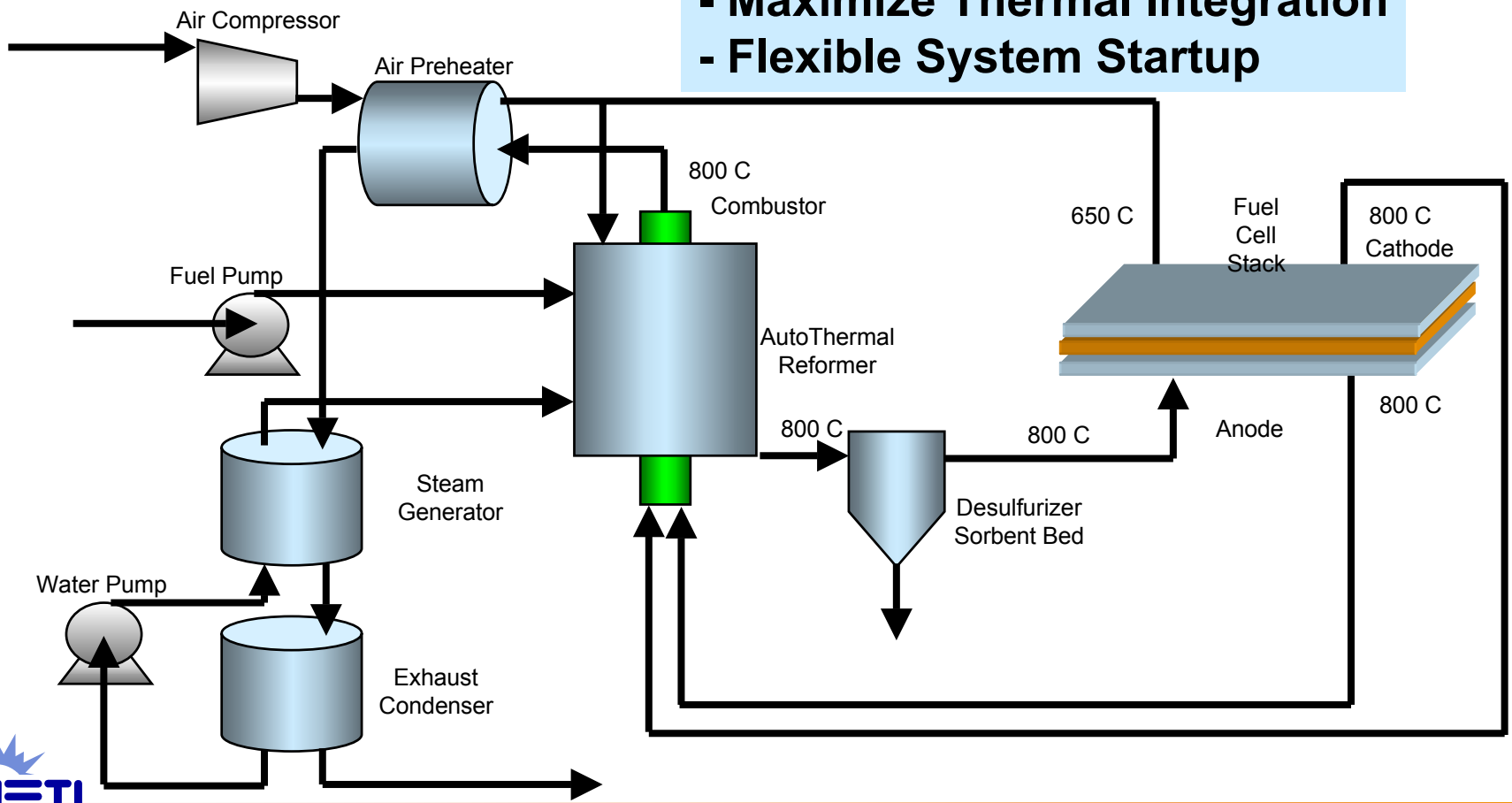
- **Conduct Kinetic Rate Determination Studies in the Laboratory to Allow for Predictive Modeling and Design**

# Diesel Fuel Processing

## *Systems Analysis - High Efficiency Integral Combustor/Reformer*

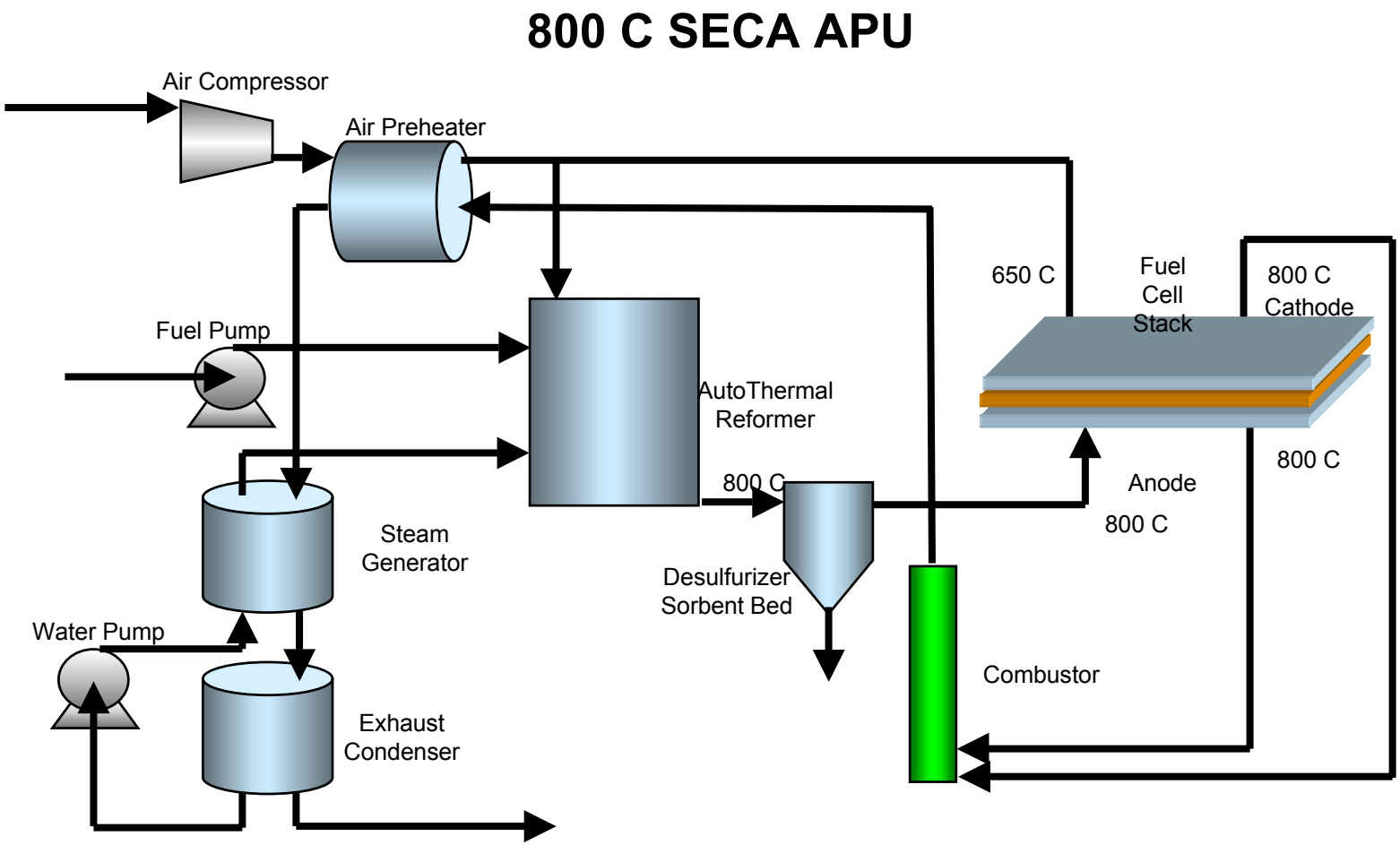
**800°C NETL APU**

**Goals:**
- **Maximize Thermal Integration**
- **Flexible System Startup**



# Diesel Fuel Processing

## *Systems Analysis - External Post Anode Combustor*



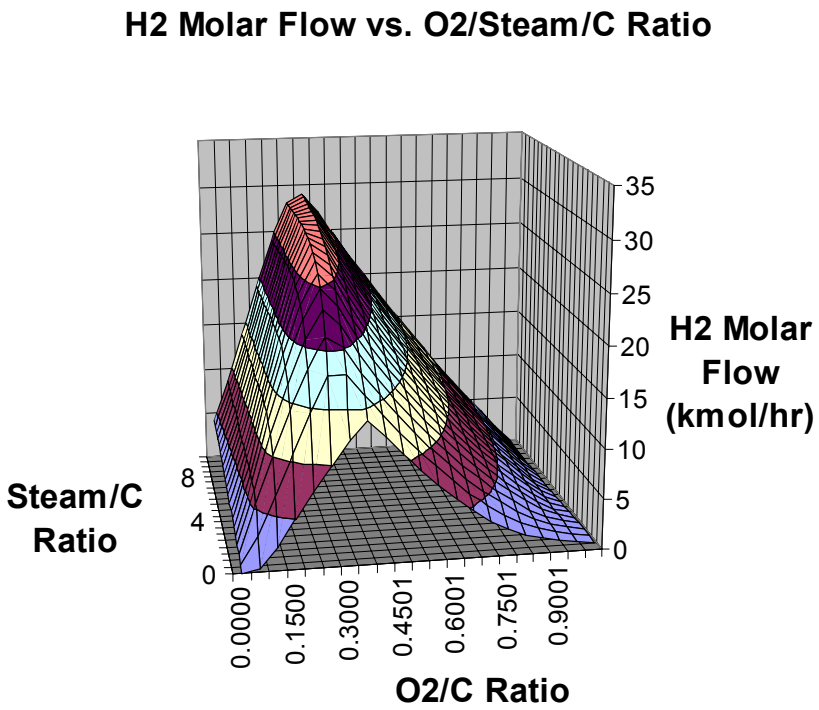
# Diesel Fuel Processing

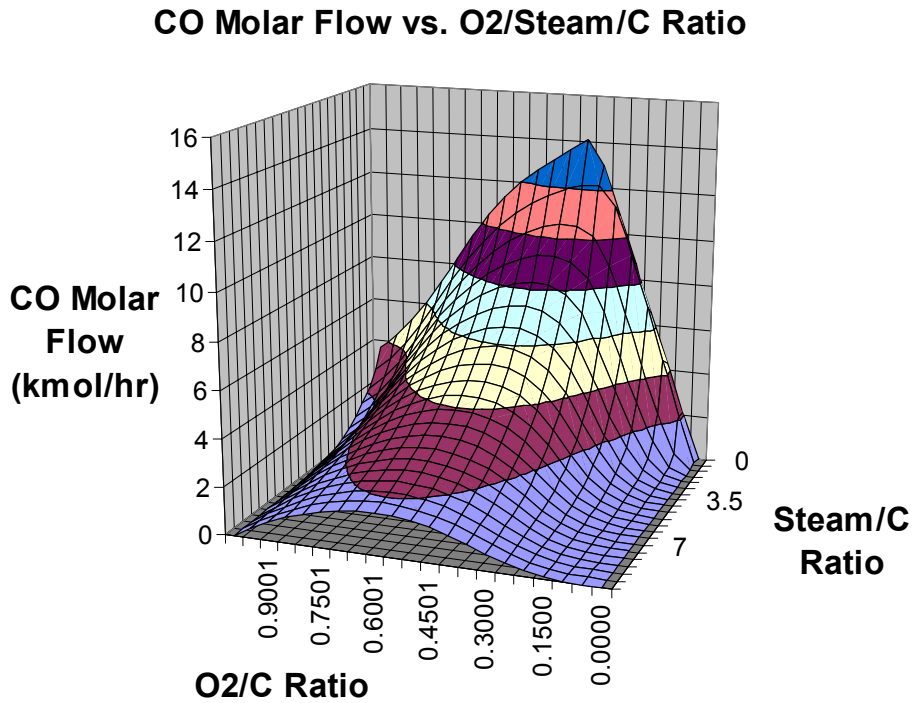
## *Systems Analysis - Effect of Heat Integration*

| | Shared Heat | Non-Shared Heat |
|---|---|---|
| Fuel (kg/hr) | 0.834 | 0.834 |
| Air – Stoichs In | 5 | 5.2 |
| ATR F/A Ratio | 9 | 3.5 |
| Steam/C Ratio | 0.8 | 0.8 |
| Efficiency | 50.21 | 42.39 |
| Net Power | 5.0 | 4.221 |
| ATR Temperature | 800 | 800 |
| FC Temperature | 865 | 813 |

# Diesel Fuel Processing

## *Systems Analysis - ATR Oxygen & Steam Sensitivity*



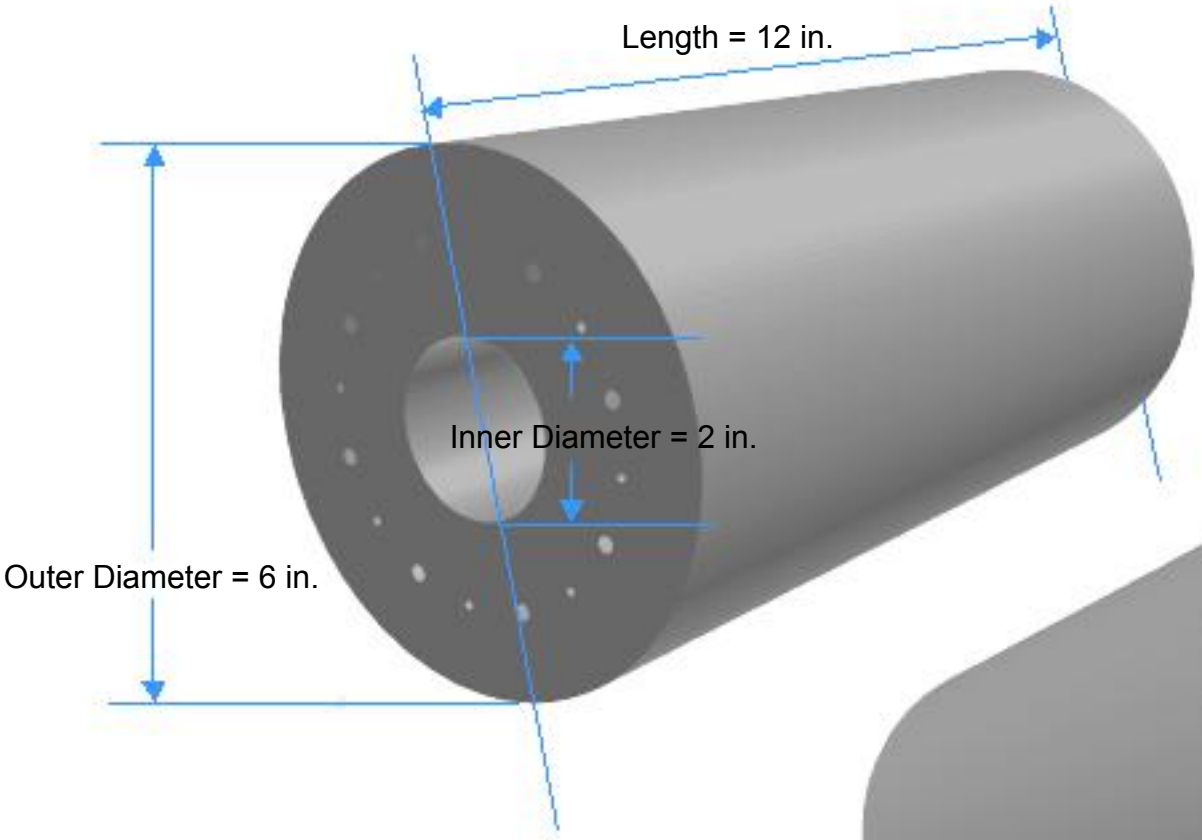



# Diesel Fuel Processing

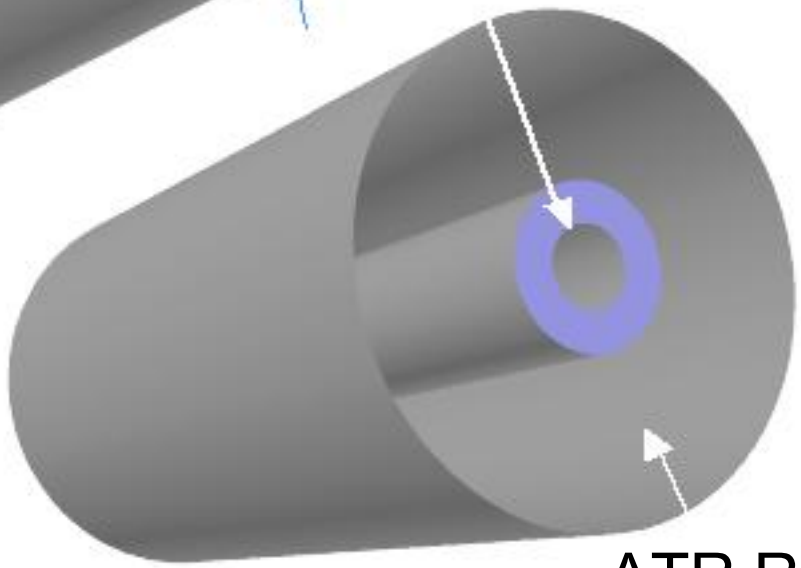
## *CFD Modeling - Approach*

- **Develop a ATR model in Fluent**
  - Fuel atomization and vaporization
  - Partial oxidation of diesel fuel
  - Combustion of anode exhaust gas
  - Steam reforming of diesel fuel
- **Obtain reaction kinetic expressions from**
  - Catalyst manufacturer
  - Literature
  - Experiments
- **Conduct steady state simulations and validate model with ATR experimental data**
- **Conduct transient simulations**
  - Use the simulation results to study reformer performance
  - Export temperature fields into ANSYS and calculate the thermal stresses

# ATR Model Prototype Geometry



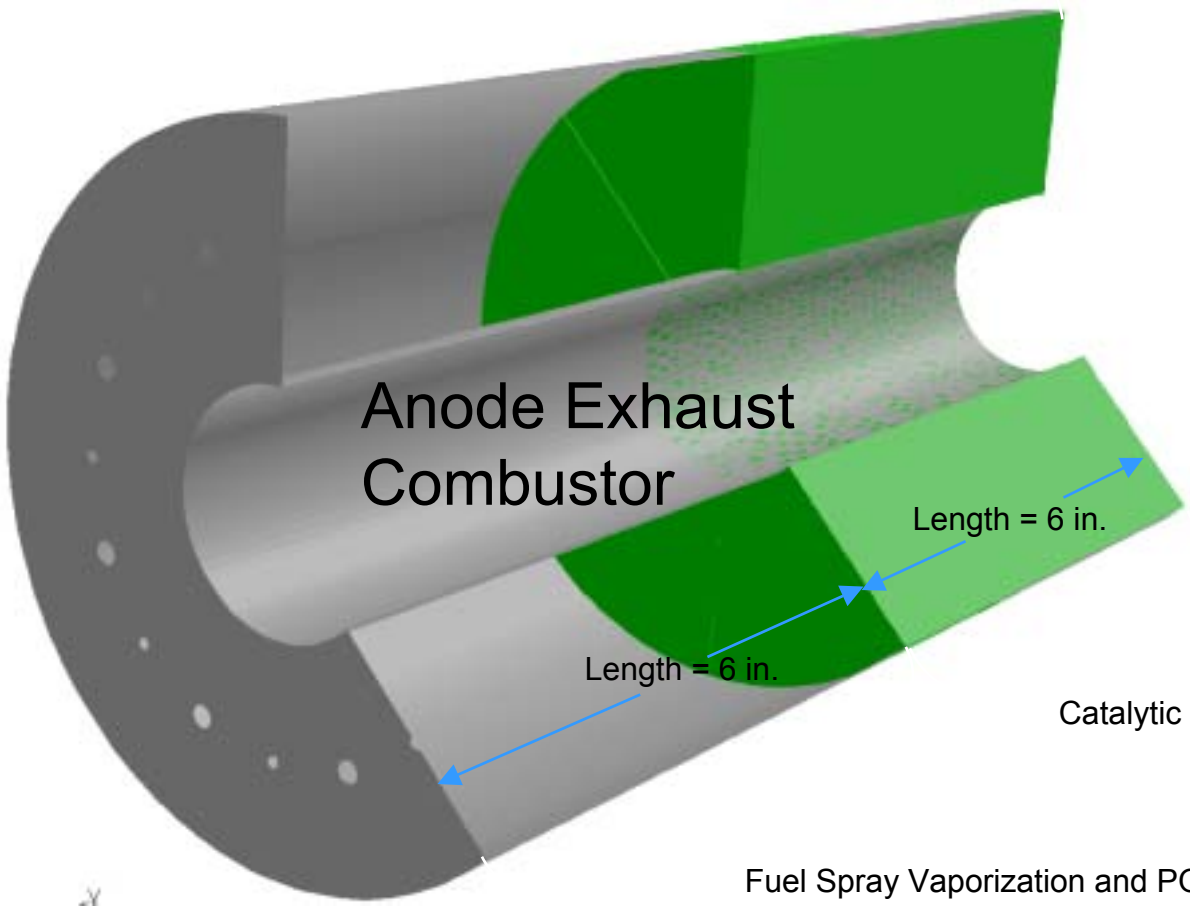

Anode Exhaust Combustor



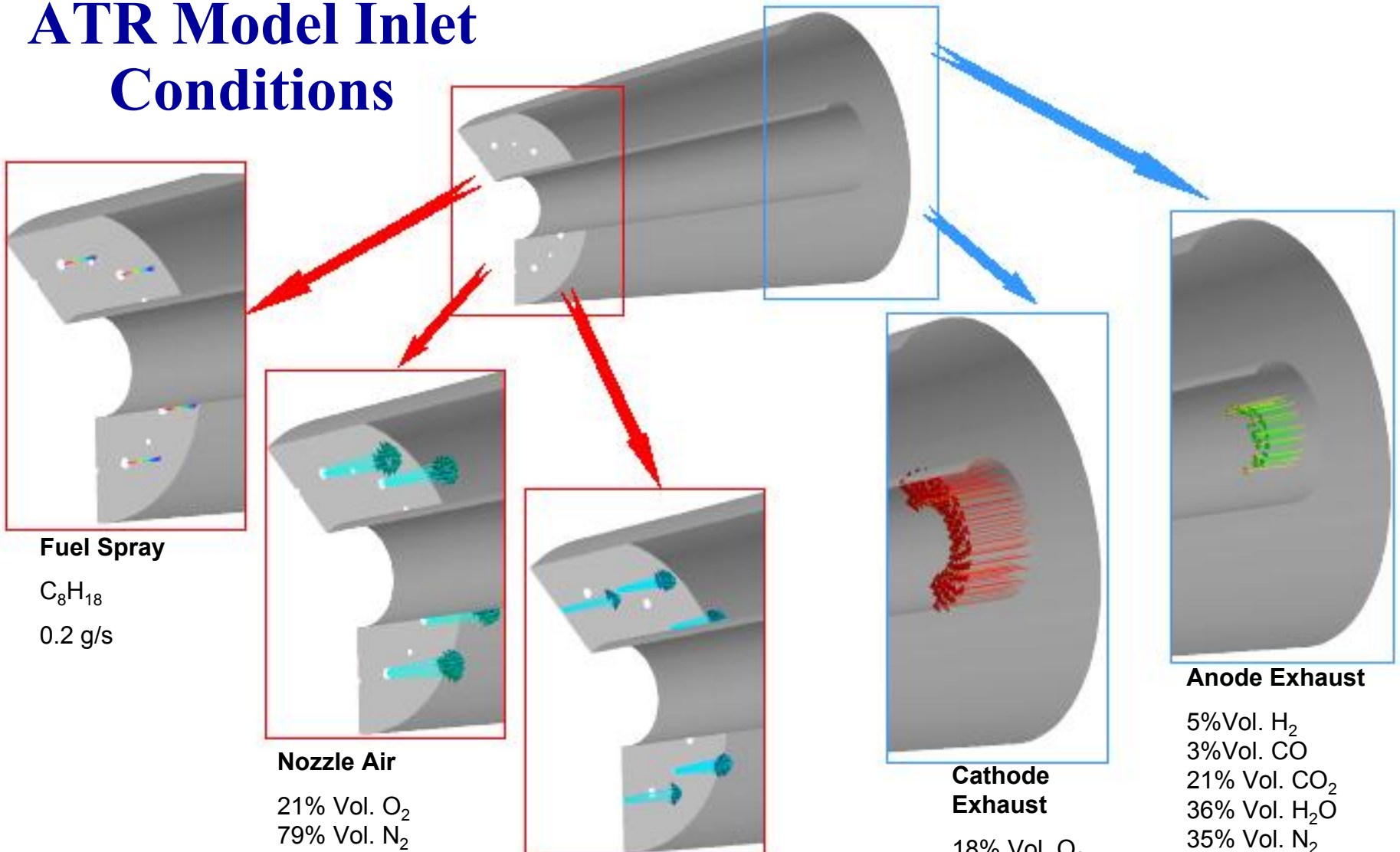
ATR Region

# ATR Model Prototype Geometry

## ATR Region



# ATR Model Inlet Conditions



**Fuel Spray**

$C_8H_{18}$

0.2 g/s

**Nozzle Air**

21% Vol. $O_2$
79% Vol. $N_2$

0.2g/s

650C/923K

**Steam**

0.18g/s

**Cathode Exhaust**

18% Vol. $O_2$
82% Vol. $N_2$
0.2g/s
650C/923K

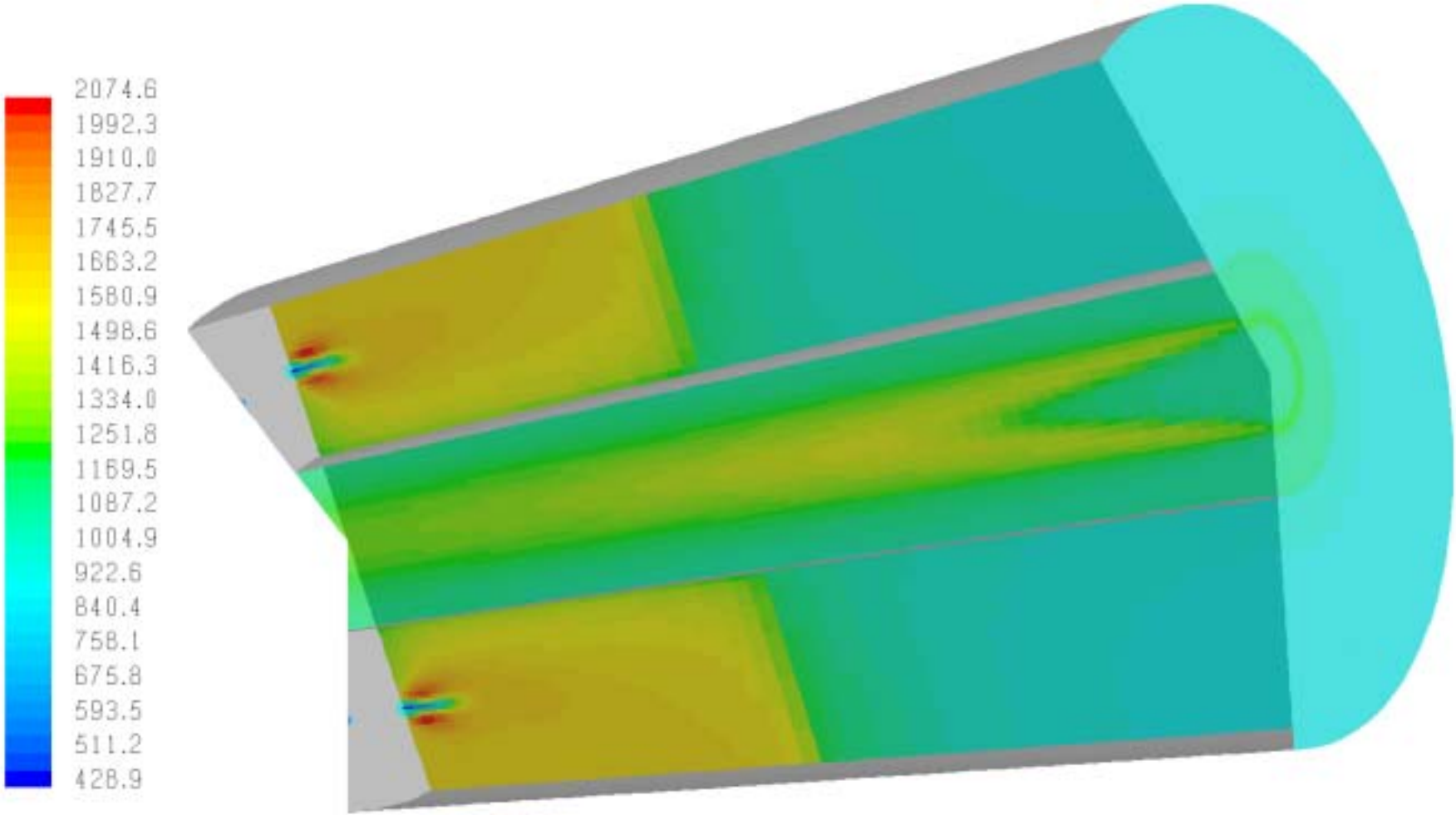
**Anode Exhaust**

5%Vol. $H_2$
3%Vol. CO
21% Vol. $CO_2$
36% Vol. $H_2O$
35% Vol. $N_2$

1.6g/s

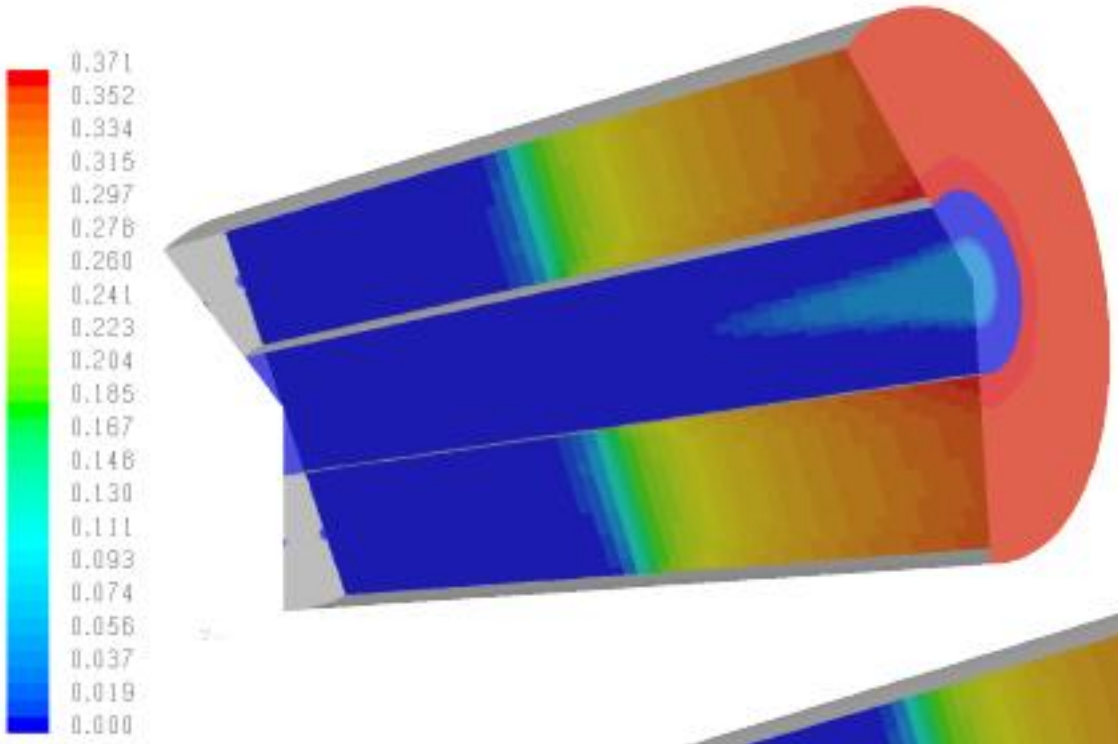
800C/1073K

# ATR Model Results

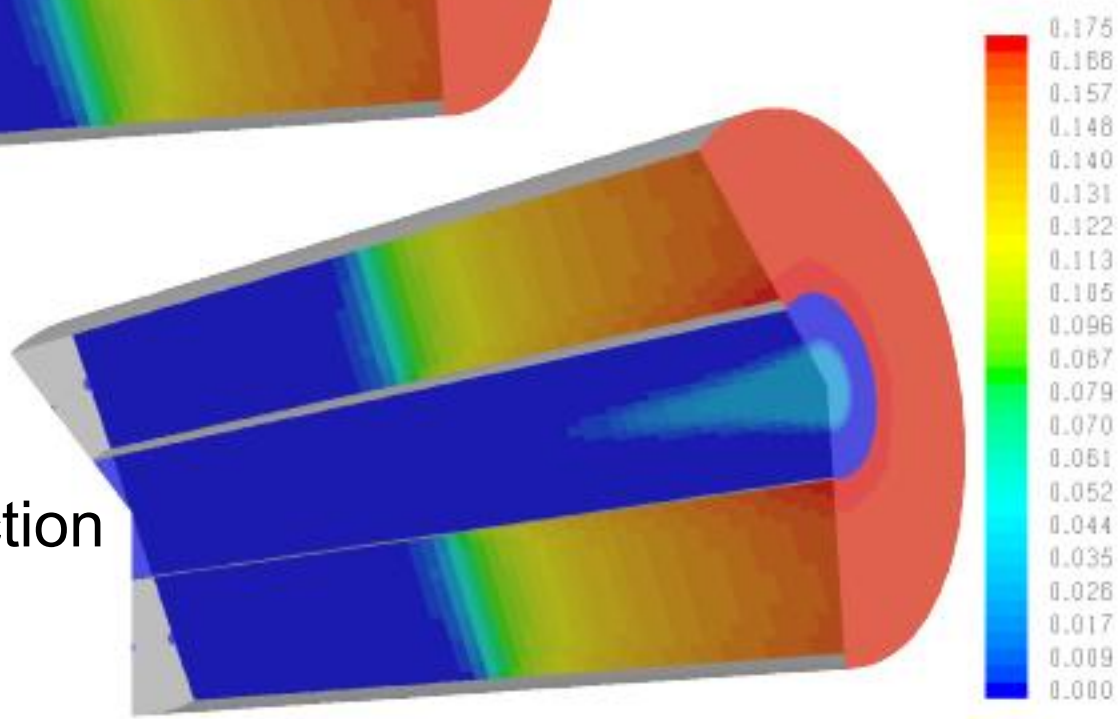



Temperature (K)

# ATR Model Results




$H_2$ Mole Fraction




CO Mole Fraction

# Diesel Fuel Processing

## *Reaction Rate Determination - Modeling Approaches*

### Level 1
**Intuitative Lumping**

- Lumps derived from intuition (gross identification of lumping groups), e.g. paraffins, aromatics, etc.
- Little is known regarding the exact mechanism
- Psuedo-1$^{st}$ order
- Psuedo-homogeneous phase
- Easy to develop, inexpensive
- Suitable for process simulators, e.g. ASPEN, ChemCad
- Predicts transient response and hydrocarbon slip

### Level 2
**Mechanism Based Lumping**

- Psuedo-homogeneous phase
- Based on psuedo-species lumped together based on the elucidation of a detailed mechanism
- Requires a knowledge of process chemistry
- Must possess the analytical ability to measure the psuedo-species only
- Suitable for process simulators, e.g. ASPEN, ChemCad
- Predicts transient response, hydrocarbon slip, coking and catalyst deactivation

### Level 3
**Structure Oriented Lumping**

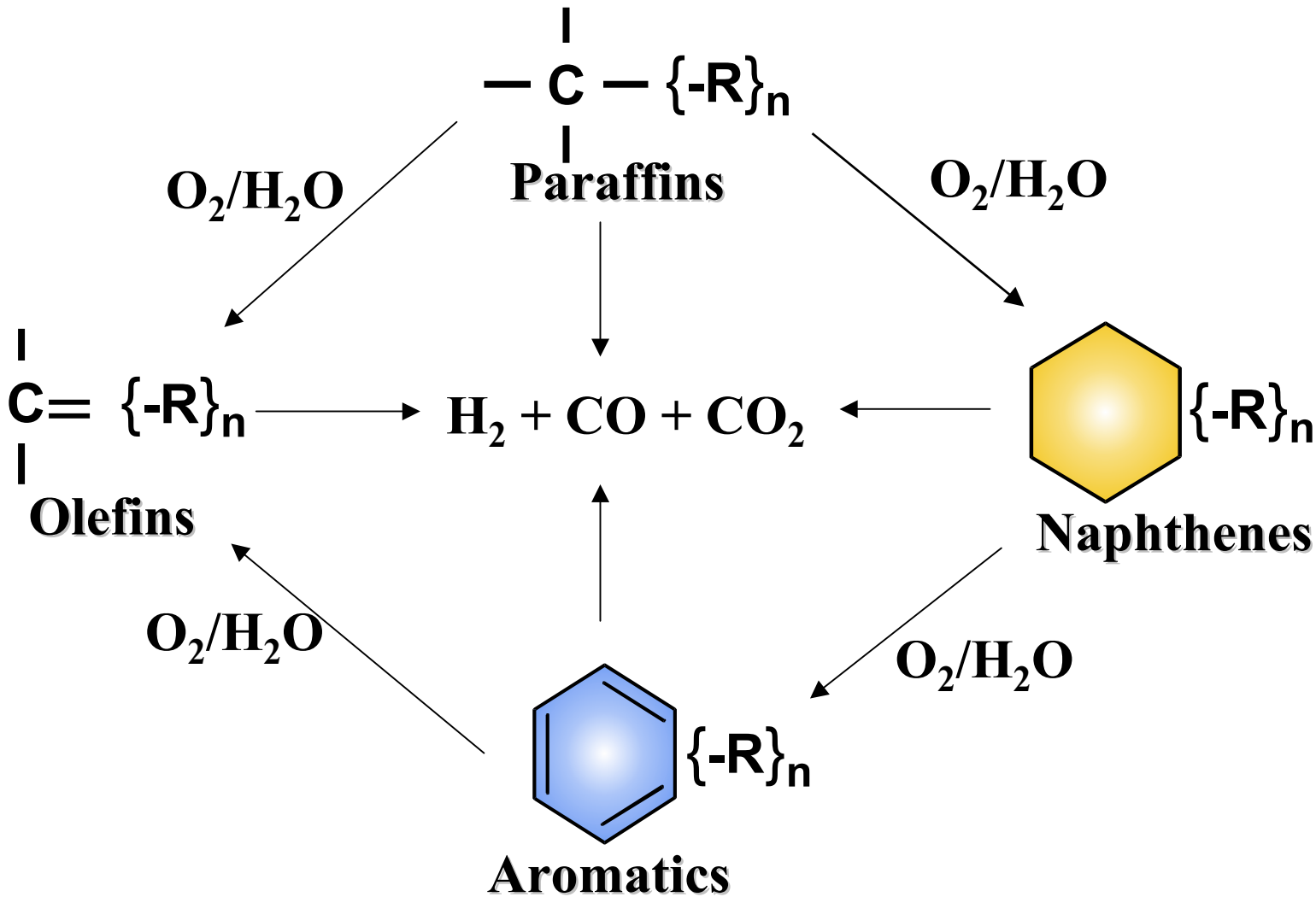
- State of the art in complex mixture modeling
- Closely resembles pure mechanistic approach
- Involves lumping isomers only
- Detailed knowledge of process chemistry needed, expensive analytically
- Detailed kinetic studies needed for the development of lumps
- Suitable for CFD packages, e.g. Fluent

### Level 4
**Mechanistic**

- Pure mechanistic approach
- Detailed kinetic studies of single components and their mixtures
- Development of experimental procedures to evaluate process chemistry
- Knowledge of catalyst properties needed
- Requires spectroscopic method
- Predicts transient response, hydrocarbon slip, coking and catalyst deactivation based on fundamentals

# Diesel Fuel Processing

## *Reaction Rate Determination - Complex Reaction Network*



# Diesel Fuel Processing
## *2002 Accomplishments*

- **Diesel-based 5-kWe fuel cell APU system with >50% electrical conversion efficiency identified**
- **A prototype CFD model including all the key elements of ATR has been developed**
  - Developed a model that accounts for fuel atomization and vaporization, partial oxidation, steam gasification, and anode exhaust gas combustion
  - Tested the convergence behavior of the model
- **Laboratory Kinetic Experiments Conducted**
  - Tested Pt, Pd, and Ru catalysts
  - Initial rate measurements made for hexadecane and diesel fuel