Reforming of Diesel Fuel for Transportation Applications

J. P. Kopasz, S. Lottes, D-J. Liu, R. Ahluwalia, V. Novick and S. Ahmed
Argonne National Laboratory

Applications of diesel fuel reforming

- Produce fuel (H_2-rich gas) for PEM and/or solid oxide fuel cells (SOFCs)
- Reduce NO_x emissions through reformate injection in internal combustion engine (ICE) and/or reformate feed to selective catalytic reduction unit

Challenges in Diesel Reforming

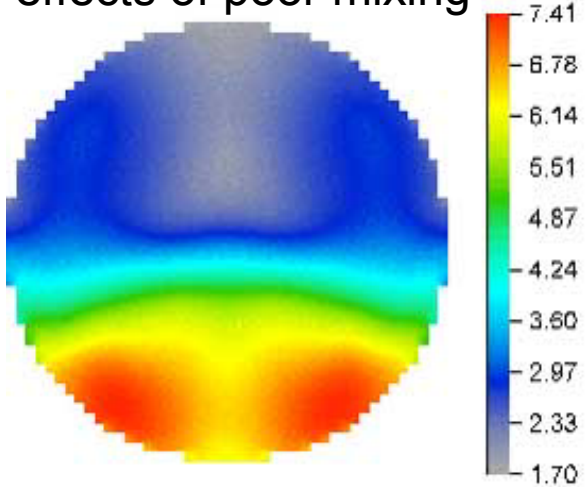
- Extending catalyst lifetime- high temperatures needed for diesel reforming degrade catalysts
- Preventing coking while maintaining high reforming efficiencies

To address these issues we are investigating

- Reactor engineering- to provide better reactant mixing, eliminate hot-spots and provide better temperature distribution
- CFD modeling of reactors
- Reforming chemistry- to determine how diesel fuel formulations, H_2O:C, and O_2:C ratios affect reforming efficiency, coking, and catalyst lifetime
- Work addresses technical barriers J, M and N

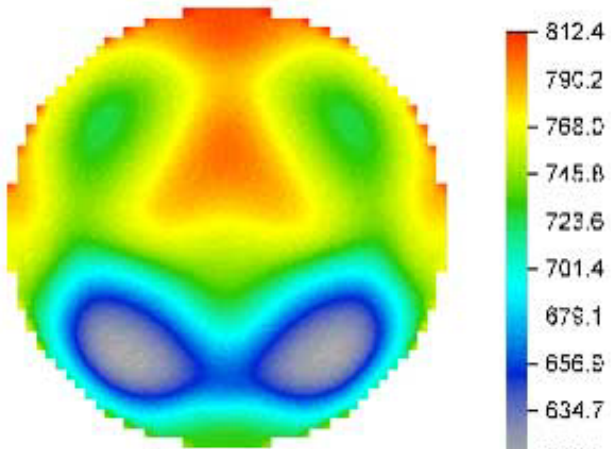
Modeling/Reactor engineering

CFD simulations show effects of poor mixing

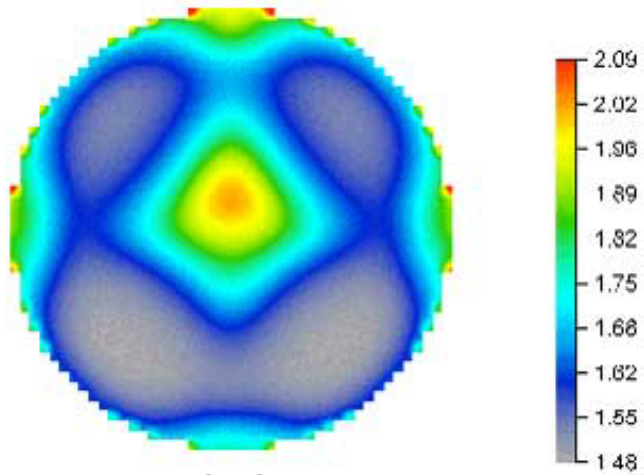


Fuel:Air Equivalence ratio

- Modeling and experiments indicate mixing of reactants is critical in avoiding hotspots and cold spots
- Proper mixing helps avoid coke formation by maintaining proper H_2O:C and O_2:C ratios



Catalyst Temperature



H_2O:C ratio

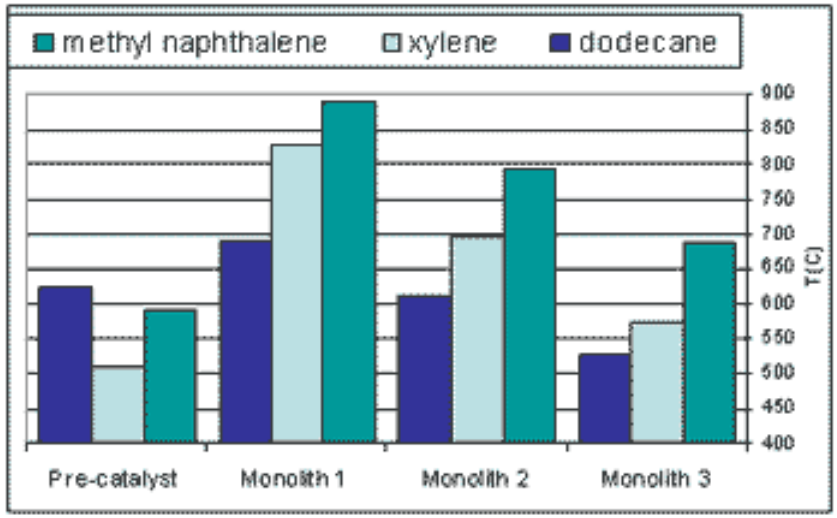
Developed injector nozzle to provide intimate mixing at reactor-relevant conditions

Developed 3- fluid injector nozzle which produces small droplets (<10μm), with low air-side pressure drop which intimately mixes fuel, steam and water prior to catalyst bed

3-fluid nozzle delivers a fine mist of fuel

Reforming Chemistry

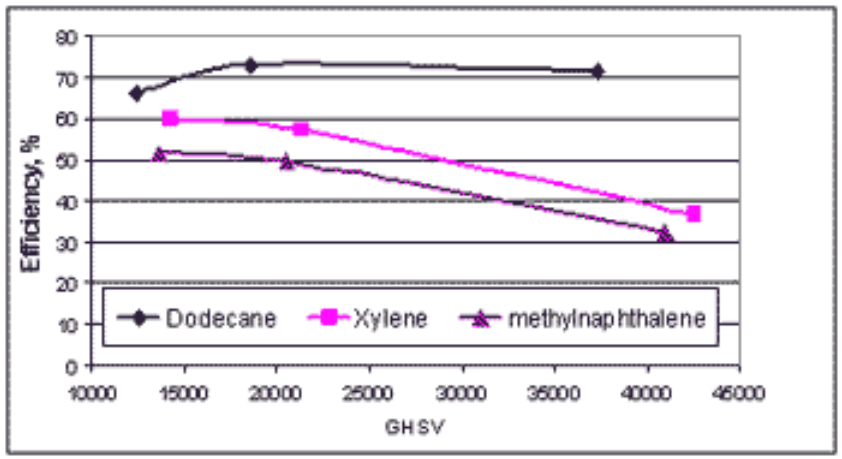
Effect of fuel on catalyst temperature



Determined effects of Fuel composition on catalyst temperature and reforming efficiency using pure component tests

Temperatures >850ºC lead to rapid catalyst deactivation

Effect of fuel on efficiency



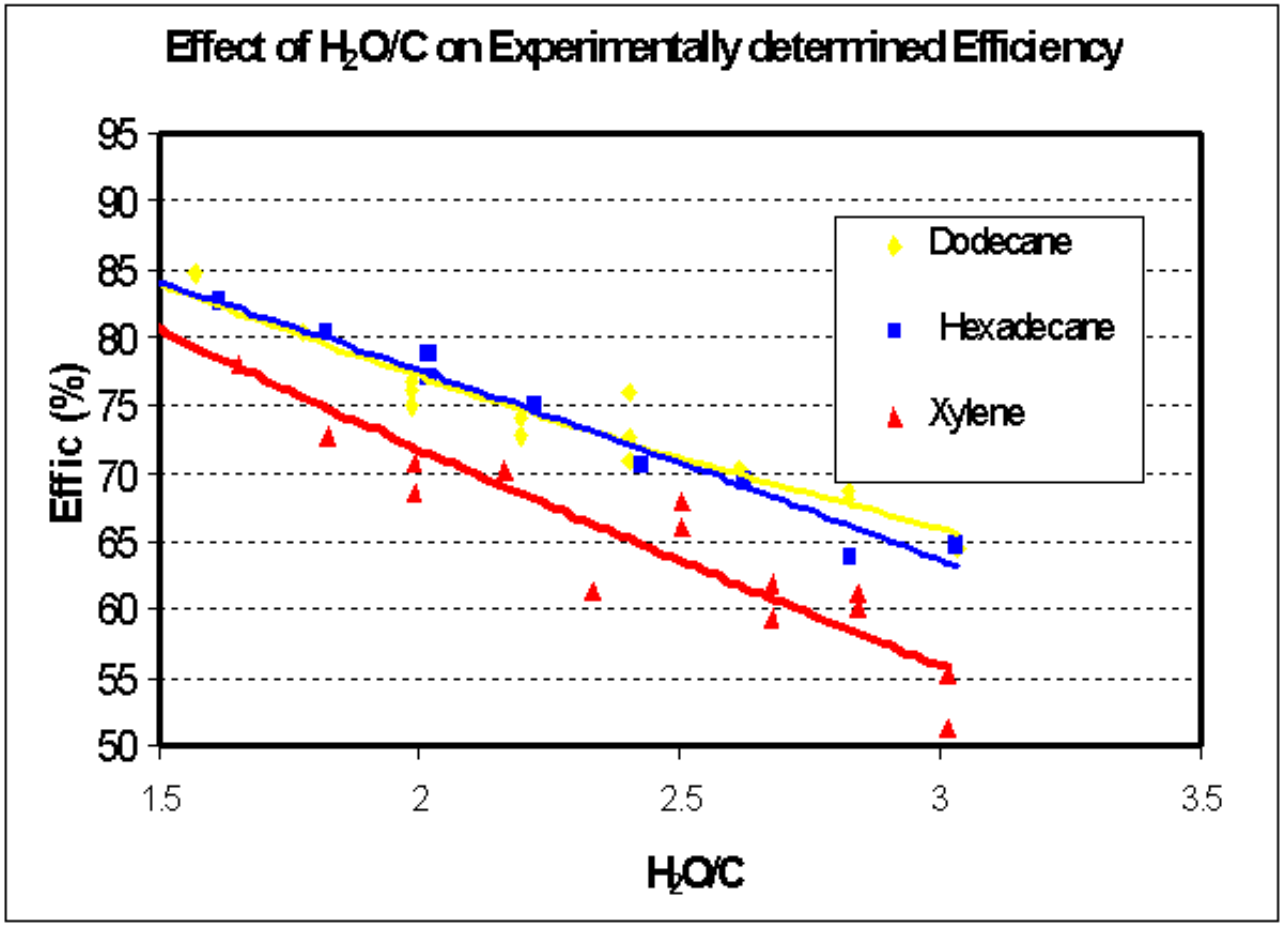
Fuel reforming efficiency to H_2 + CO, ηref

$$\eta ref = \{ct,_{H2}\Delta Hc,_{H2} + ct,_{CO}\Delta Hc,_{CO}\}/ct,_{fuel}\Delta Hc,_{fuel}$$

Ct,i = Molar flow rate of i

$\Delta Hc,i$ = Heat of combustion of i

Effect of Increasing H_2O:C Ratio



- To avoid coking, many reformers are run at high H_2O:C ratios
- Increasing H_2O:C has a negative impact on conversion efficiency

Conclusions/Accomplishments

- Proper delivery and mixing of reactants are needed to obtain high efficiencies and avoid hot spots and areas of low H_2O:C and O_2:C ratios
- Demonstrated operation of liquid fuel injector
- Determined substantial differences in reforming of different diesel fuel constituents
  - Aromatics result in higher maximum reforming temperatures and lower energy conversion efficiencies
  - *Di-aromatics are more difficult to reform than mono-aromatics.*
  - *Increasing H_2O:C ratio reduces coking but decreases overall efficiency*

Future Plans

- Determine how fuel composition affects catalyst durability
- Investigate reforming under POX conditions and in low H_2O:C regimes
- Collaborate with NETL (modeling efforts)