Effects of Fuel Composition on Fuel Processing

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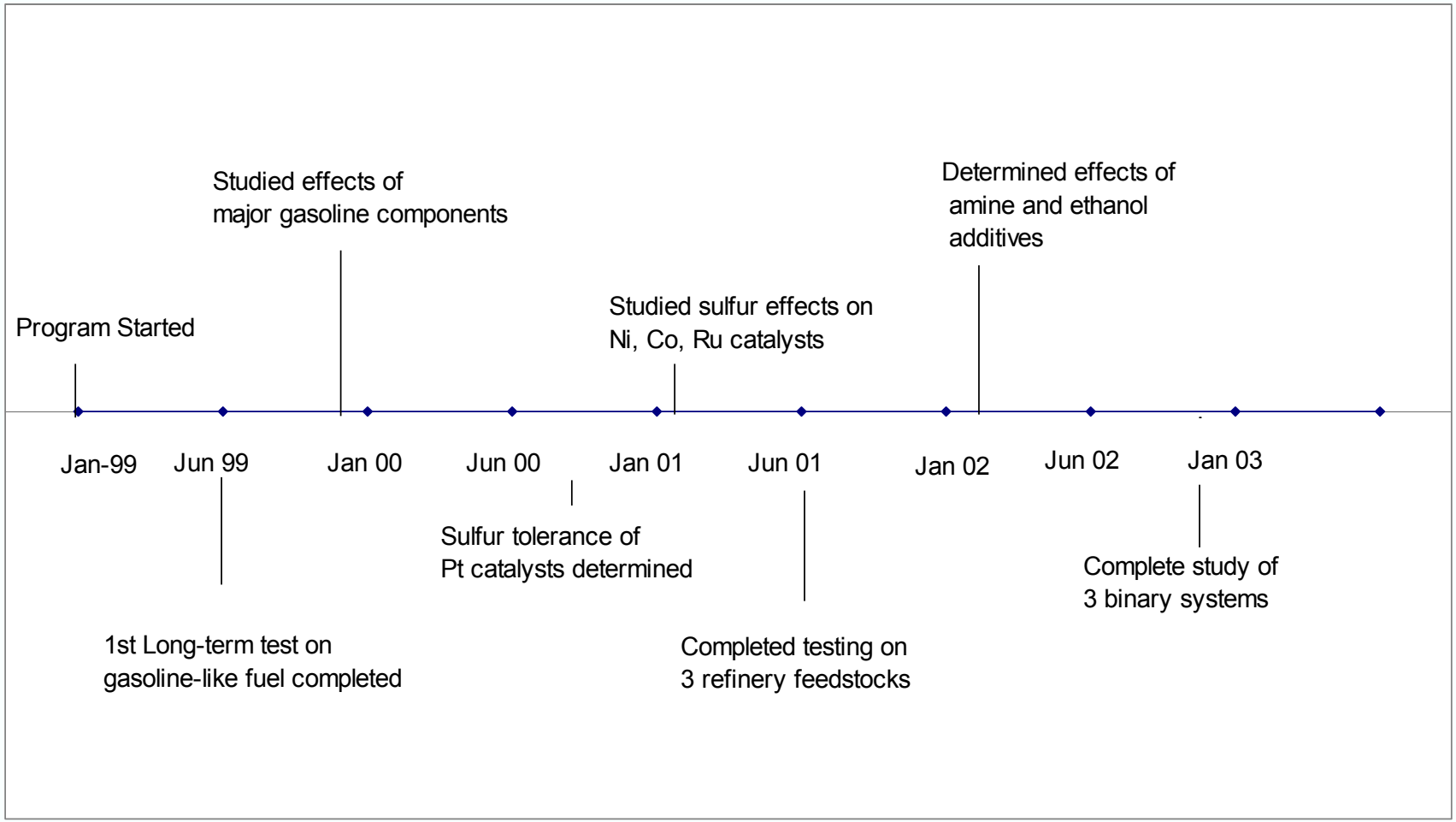
Objective:Evaluate petroleum-based fuels for fuel cell vehicles

- Determine effects of major constituents, additives, and impurities in petroleum fuels on fuel processor performance and durability
- Collaborate with major oil companies for development of future fuels for fuel cells

Timeline


Studied effects of
major gasoline components
Determined effects of
amine and ethanol
additives
Program Started
Studied sulfur effects on
Ni, Co, Ru catalysts
Jan-99
Jun 99
Jan 00
Jun 00
Jan 01
Jun 01
Jan 02
Jun 02
Jan 03
Sulfur tolerance of
Pt catalysts determined
Complete study of
3 binary systems
1st Long-term test on
gasoline-like fuel completed
Completed testing on
3 refinery feedstocks

Industrial interactions

- Interacting with 3 major oil companies
  - Oil companies providing
    - Input/advice on experimental plans
    - Refinery blends and real-world fuels to test
    - Additional insight for data interpretation
    - Performing testing using different catalyst forms
    - Kinetics/reactor modeling

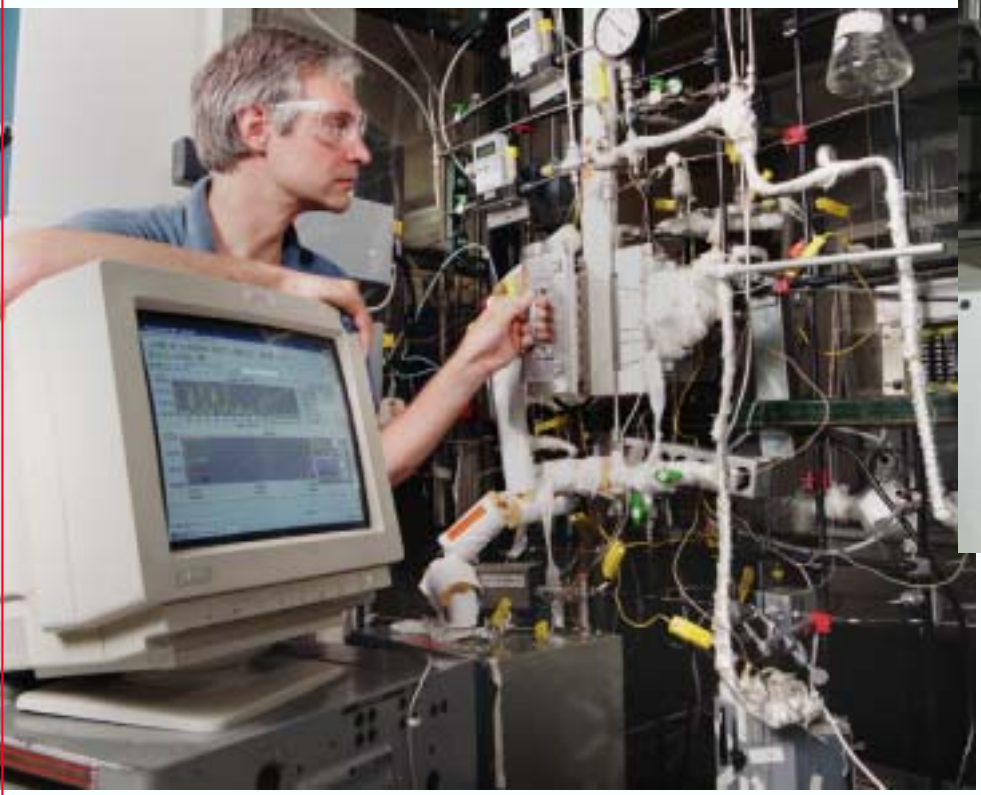
Fuel composition affects many performance targets

- Fuel processor efficiency (80%)
- Processor durability (> 5000 h)
- Operational GHSV (>200,000 h^{-1} for ATR)
- Catalyst volume
- Catalyst weight
- Refueling infrastructure costs

Experimental approach

- Determine product gas composition dependence on temperature and space velocity using a microreactor (relates to targets for reforming efficiency, and GHSV)
  - test major fuel components individually
  - test minor components, additives, and impurities as isooctane solutions
  - test blends of fuel components
- Long-term testing (1000h)
  - determine poisoning, long-term degradation effects

Experimental apparatus- Short and long term test reactors

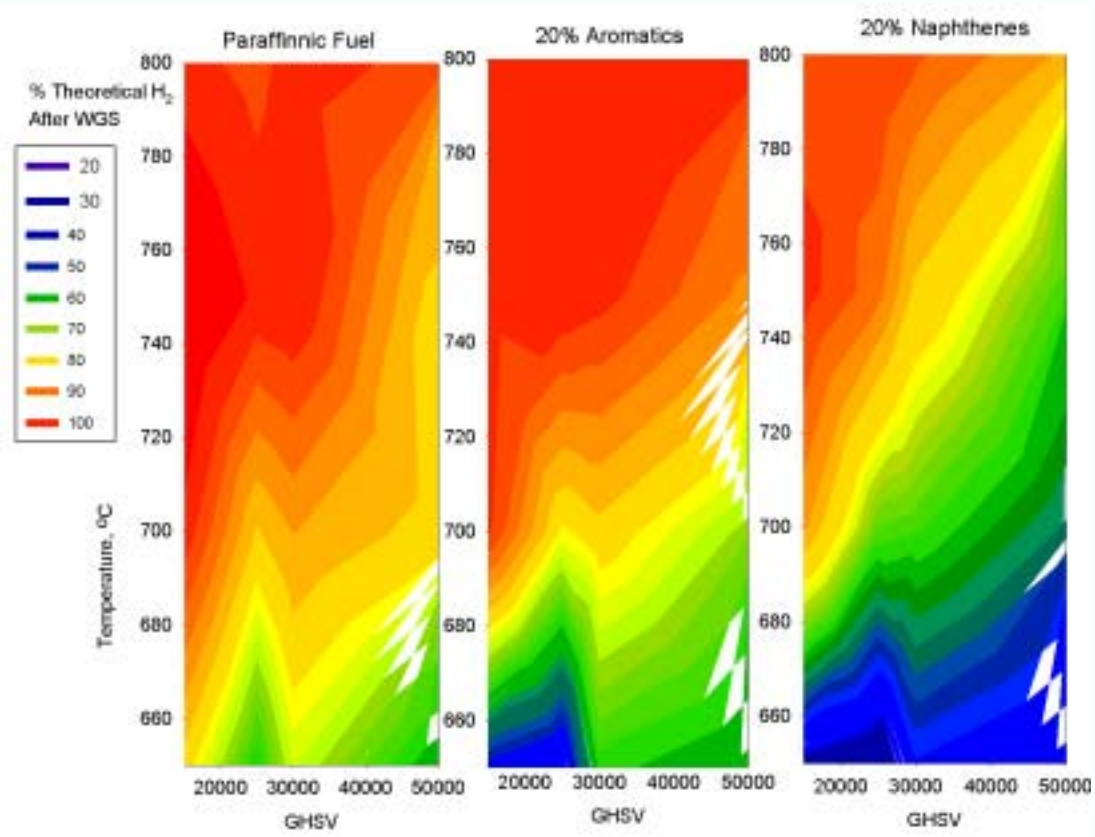


Highlights

- Paraffinic fuels reform more readily
- Aromatics and naphthenes affect the rate at which paraffinic fuels are reformed
- Detergent additives affect rate at which paraffinic fuels are reformed
- Fuel composition affects the water balance in the fuel cell system

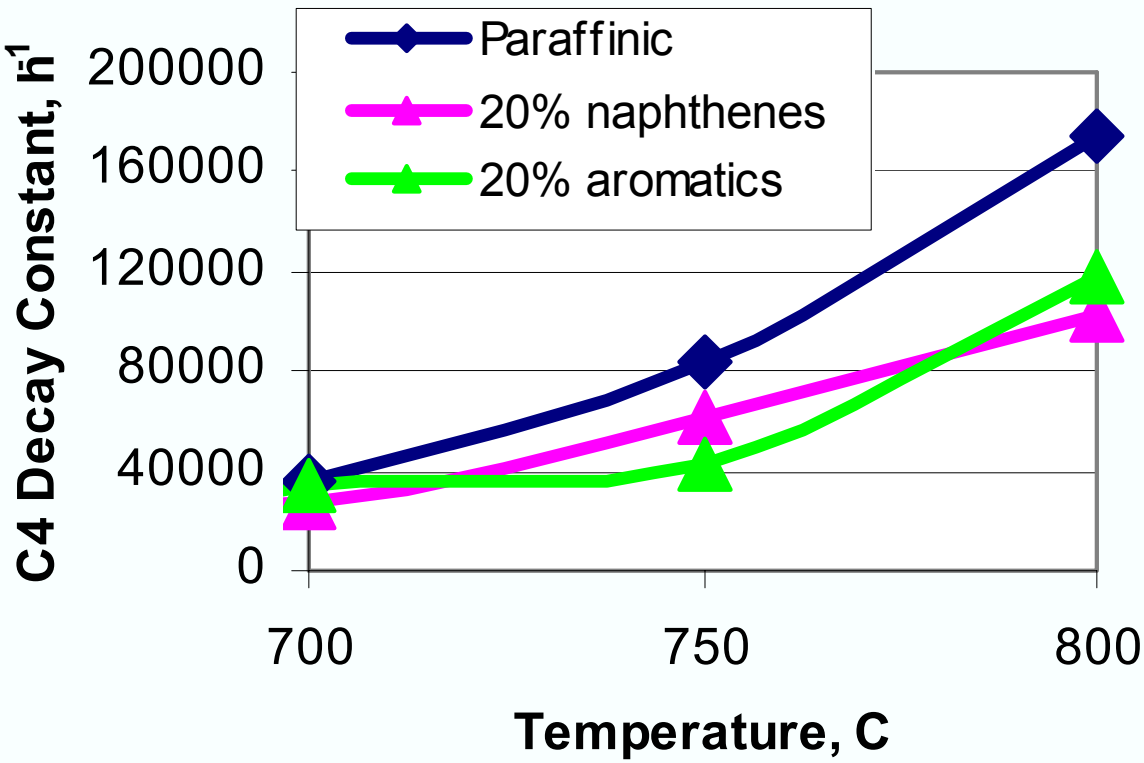
Real-world fuels containing aromatics or naphthenes perform poorer than paraffinic fuels

- Fuel with 20% aromatics performed poorer at low temperature
- Fuel with 20%naphthenes performed poorer at low temperature or high GHSV



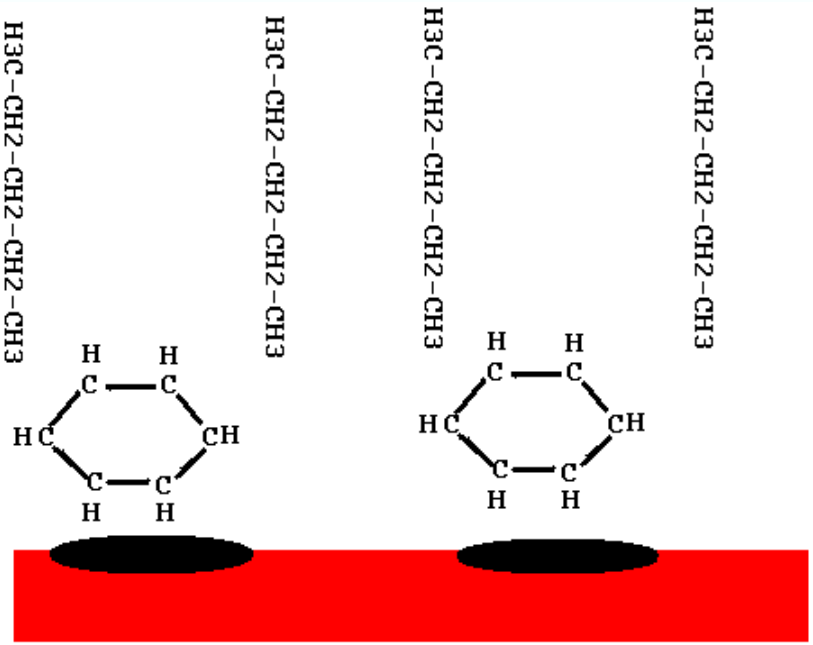
Aromatics and naphthenes inhibit the reforming of paraffins

- Aromatics or naphthenes decreased the rate of destruction of C4 species



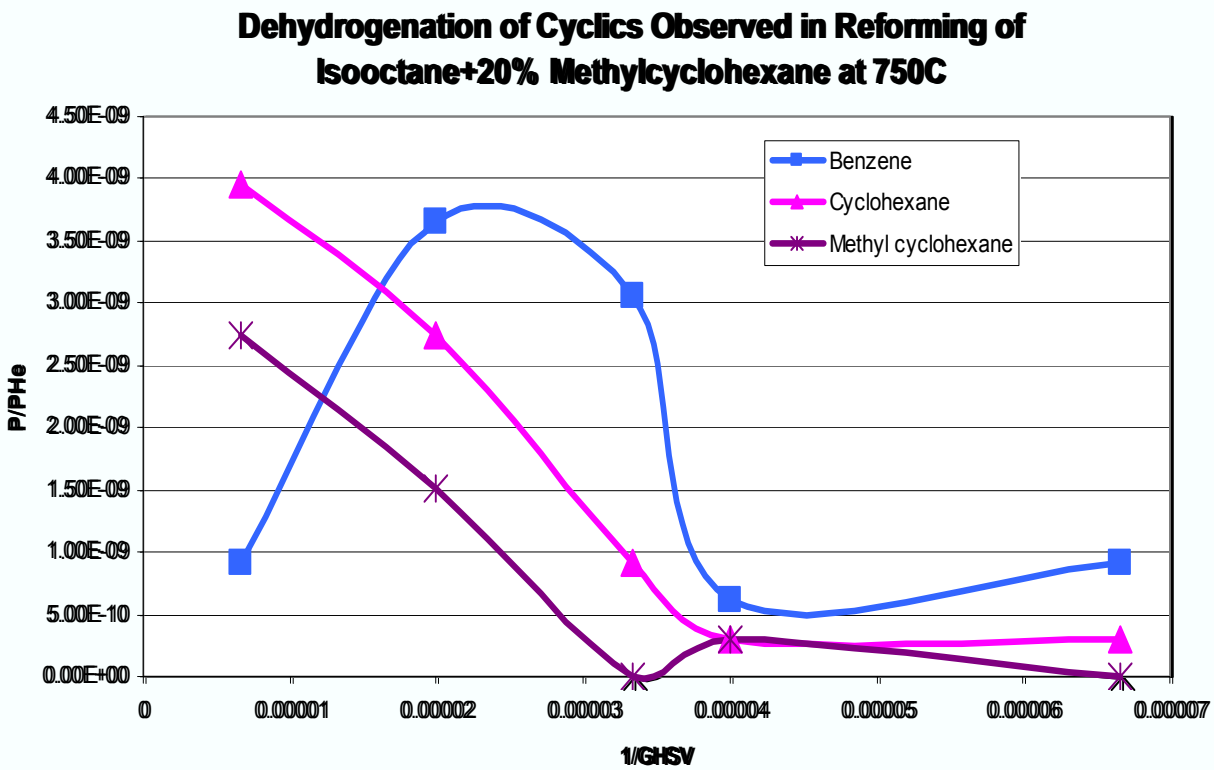
Aromatics poison reaction sites

- Aromatics bind more strongly to the metal centers
- Aromatics react more slowly at the metal center
- Results in lower reaction rates for paraffinic species



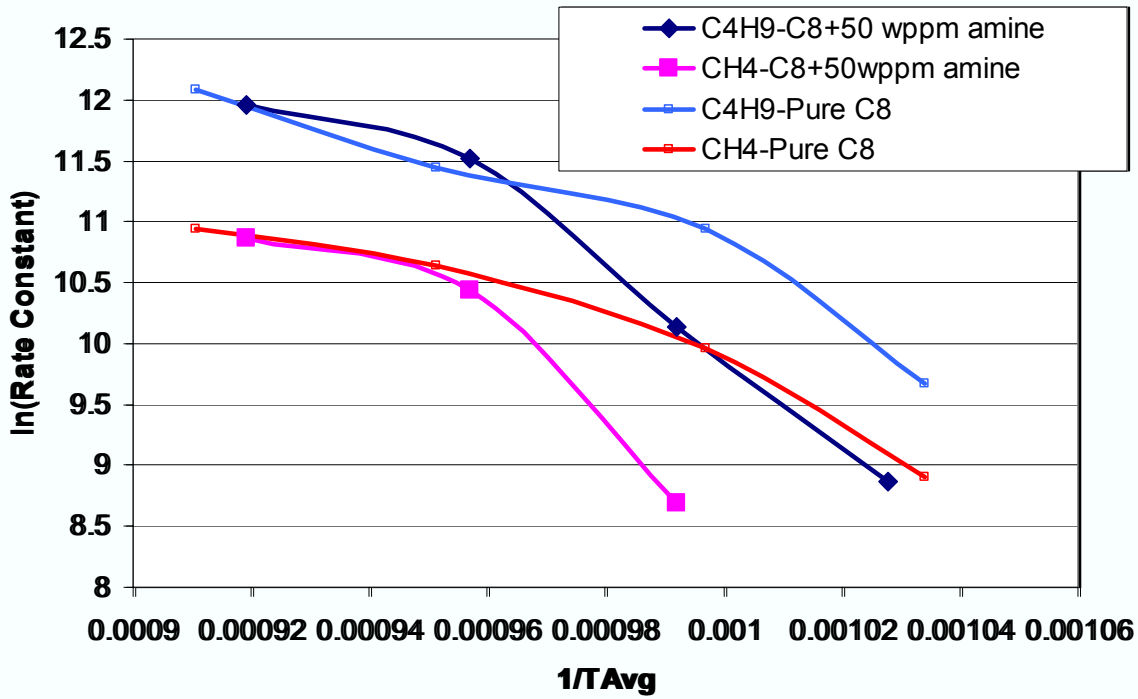
Naphthenes lead to formation of aromatics which are detrimental

- Dehydrogenation occurs in initial stages of naphthene reforming.
- The aromatics formed from dehydrogenation then poison catalyst sites



Amines used in gasoline additives affect reforming behavior

- Detergent surrogates decrease the rate of reforming of paraffins at lower temperatures, but have little affect at higher temperatures
- No ammonia observed in product gas with up to 500 wppm n-secbutyl amine at 800°C (<250 ppb)



Fuel composition has an effect on water requirements

Fuel	Gasoline	Isooctane	Trimethyl-benzene	Toluene
Water Needed for reforming (moles H_2O/moles H_2 produced)	0.71	0.67	0.79	0.82
Exhaust Temperature needed for water balance °C (°F)	42.0 (107)	43.2 (109)	36.6 (97)	34.5 (93)

Calculations for system with a temperature rise of 200°C in reformer, a radiator approach temperature of 11°C, and identical H_2O:C ratio of 1.5

Conclusions

- Fuel composition impacts the operating temperature and GHSV
- Species which are adsorbed strongly at the metal center, such as aromatics and amines, decrease rate of reforming of paraffins
- Fuel composition affects the water balance of the fuel-cell system

Milestones

- Complete short term tests on the effects of 2 additives on the reforming of isooctane 2/02
  - Status-Completed tests on n-secbutyl amine (detergent surrogate) and ethanol (oxygenate)
- Complete tests on the reformability of 3 binary fuel systems due 9/02

  Aromatic-paraffin

  Naphthene-paraffin

  Aromatic-naphthene
  - Status- ongoing

Future Work

- Determine effects of antioxidant additives
- Study long-term effects of additives
- Investigate tailored refinery blends
- Investigate water-recovery issues with refinery fuels