Supercritical Fuel Pyrolysis

Judy Wornat

Louisiana State University
Department of Chemical Engineering
Baton Rouge, Louisiana
U. S. A.

Supercritical Conditions for Fuels in Next-Generation High-Speed Aircraft

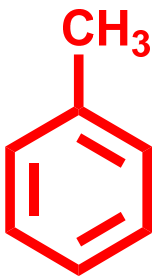
FUEL USED AS A COOLING AGENT IN HIGH-SPEED AIRCRAFT

HIGH PRESSURES AND HIGH TEMPERATURES SUSTAINED IN THE FUEL LINES

PYROLYTIC REACTIONS PRODUCE POLYCYCLIC AROMATIC HYDROCARBONS (PAH), PRECUR-SORS TO CARBONACEOUS SOLID DEPOSITS

TO UNDERSTAND THE REACTION CHEMISTRY, SUPERCRITICAL PYROLYSIS EXPERIMENTS ARE PERFORMED WITH MODEL FUELS

Model Fuels



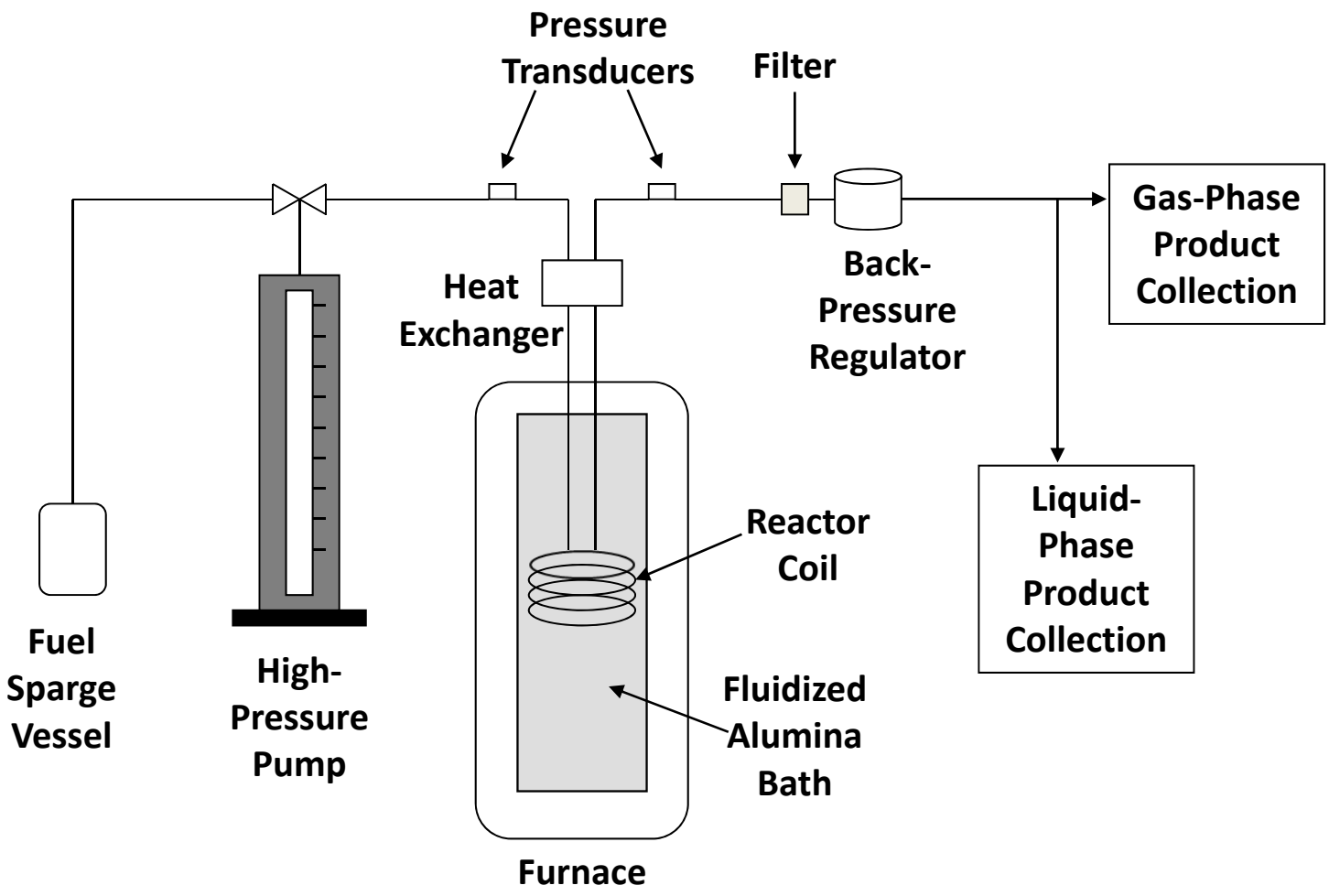
toluene

T_c = 319 °C
P_c = 41 atm

n-decane

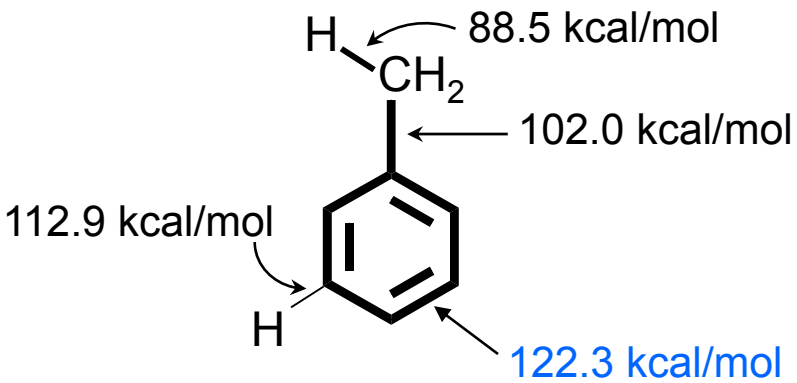
T_c = 345 °C
P_c = 21 atm

Supercritical Fuel Pyrolysis Reactor System



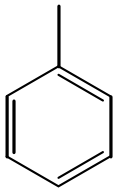
Results from Supercritical Toluene Pyrolysis at T ≤ 700 ^{0}C

- Gaseous products: > 95% methane, some ethane, and trace amounts of others; no acetylene. **No rupture of the aromatic ring**.
- Bond-dissociation energies [Luo (2003); Sanderson (1976)]:

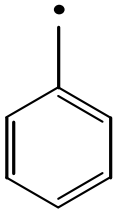


- PAH formed by reactions involving:

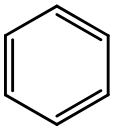
toluene



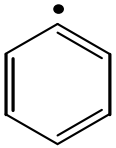
benzyl



benzene



phenyl



methyl

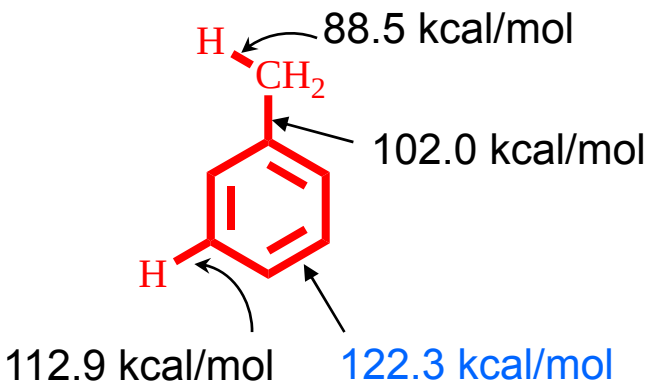
$\bullet CH_3$

hydrogen

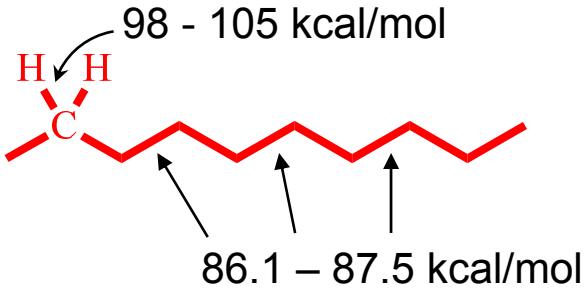
$\bullet H$

Model Fuels

Toluene



***n*-Decane**



Summary: Supercritical *n*-Decane Pyrolysis

Supercritical *n*-decane pyrolysis experiments conducted at 570 °C, 140 sec, and at six pressures from 40 to 100 atm.

PAH products identified and quantified by normal-phase HPLC fractionation / reversed-phase HPLC analysis.

One- to nine-ring aromatic product yields quantified as functions of pressure.

PAH product yields adhere well to first-order global kinetic behavior.

Pressure-dependent global kinetic rate parameters $\Delta V^{\neq}$ and A determined for 31 unsubstituted and 26 alkylated aromatic products.

Activation volumes at 570 °C : -2.4 L/mole for benzene; -3 to -8 L/mole for PAH; generally the highest magnitudes exhibited by the large PAH, the precursors to solid deposits, demonstrating the extreme pressure-sensitivity of their rates of formation.

Acknowledgements

Air Force Office of Scientific Research.

Sean Bagley, Khue Nguyen, Venky Kalpathy.

Anyone interested in finding out more about this work can contact the principal investigator:

Professor Mary Julia (Judy) Wornat
Louisiana State University
Department of Chemical Engineering
South Stadium Drive
Baton Rouge, Louisiana 70803

(225) 578-7509
mjwornat@lsu.edu