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Experimental and Kinetic Modeling Study of Ethanol Combustion at High Pressures and Intermediate Temperatures

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Introduction

A series of experimental and numerical investigation into ethanol oxidation at high pressures and intermediate temperatures has been done. The experiments, with ethanol and oxygen highly diluted in nitrogen, were carried out in a high pressure laminar flow reactor at 50 bar pressure and a temperature range of 600−900 K. The fuel-air equivalence ratio of the reactants was varied in the range of 0.1−43, i.e. from oxidizing to strongly reducing conditions. The total flow rate of the reactor was kept constant and temperature and residence time of the reactor were changed.

Furthermore, a reaction mechanism based on the previous model by the current research group is developed. Selected rate constants have been updated according to new measurements or calculations, and the general pressure dependency format for the pressure dependent reactions has been used widely. In addition to modeling of the present experiments, the mechanism is used to simulate other published data on ignition delay time and laminar burning velocity of ethanol.

Experimental Setup – Laminar Flow Reactor

- Quartz reactor to minimize surface reactions
- Steel pressure shell to achieve high pressures
- Temperature: 600–900 K
- Pressure: 50 bar
- Flow: 4.78 NL/min
- Isothermal Zone: 40–44 cm
- Residence time: 4.0–6.4 s
- Measurement via 6890N Agilent GC: O_2, CO, CO_2, light hydrocarbons, alcohols, and DME

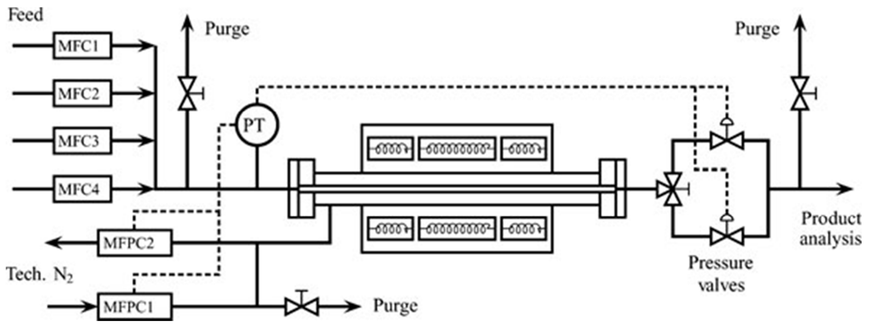

Fig 1. Schematic diagram of the high pressure laminar flow reactor

Reaction Kinetics Model

- Developed based on the previous mechanism [1]
- Updated in accordance with new measurements and calculations, e.g., H_2/O_2 subset and ethanol reactions subset [2]
- 986 reactions and 136 species
- Solution via *Chemkin-Pro*

Results

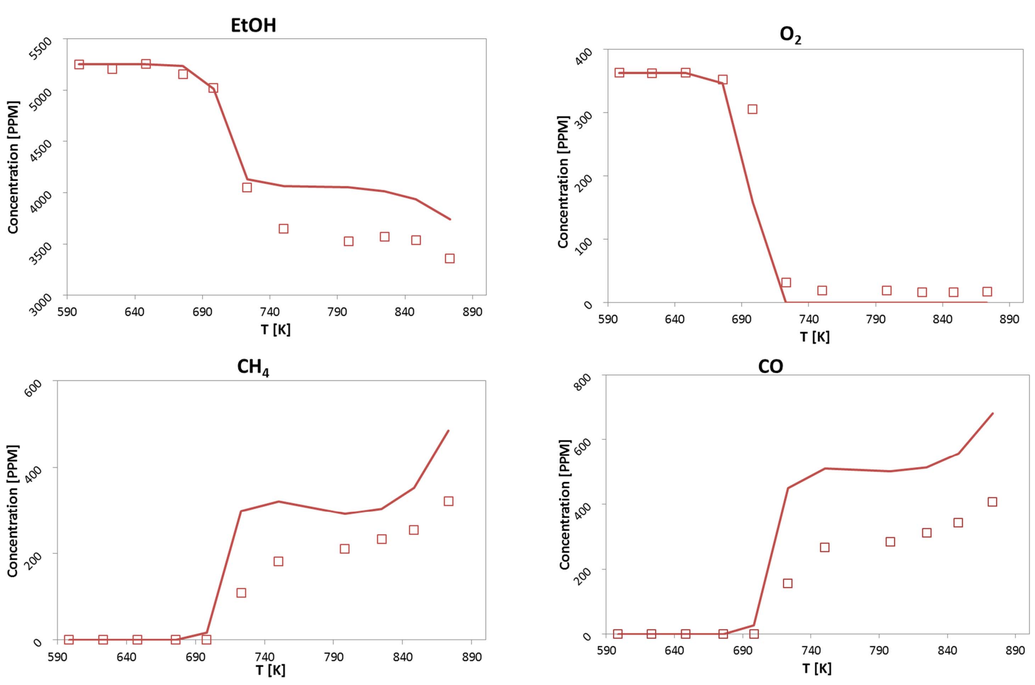

Fig 2. Results of reducing experiments in the flow reactor (0.525% ethanol and 0.0363% O_2 in N_2, Φ=43.4) at 50 bar pressure.

Results- Continued

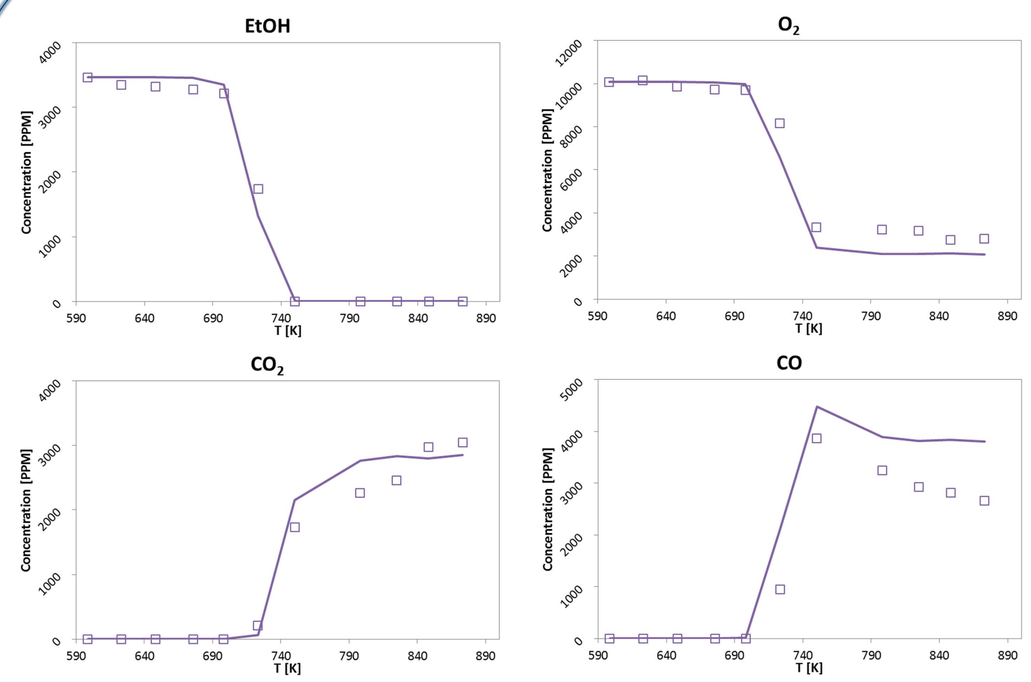

Fig 3. Results of stoichiometric experiments in the flow reactor (0.347% ethanol and1.008% O_2 in N_2, Φ=1.0) at 50 bar pressure.

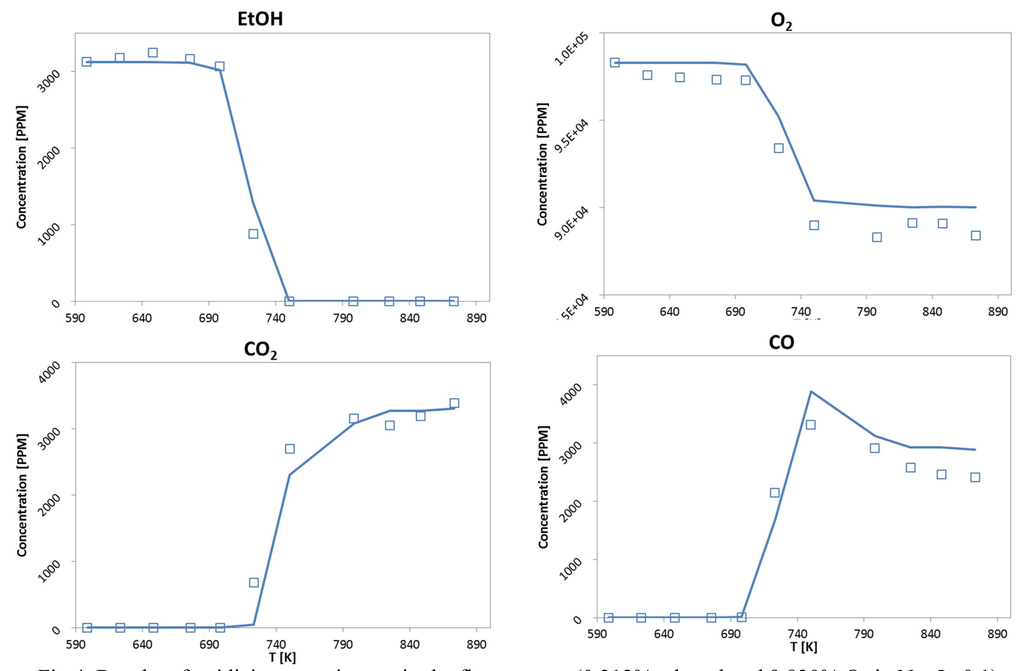

Fig 4. Results of oxidizing experiments in the flow reactor (0.312% ethanol and 9.830% O_2 in N_2, Φ=0.1) at 50 bar pressure.

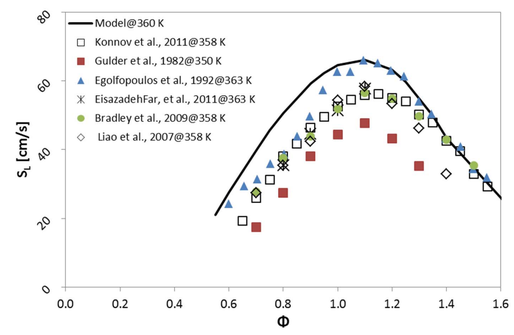

Fig 5. Laminar burning velocity of EtOH/Air at atmospheric pressure, measurements from [2-8].

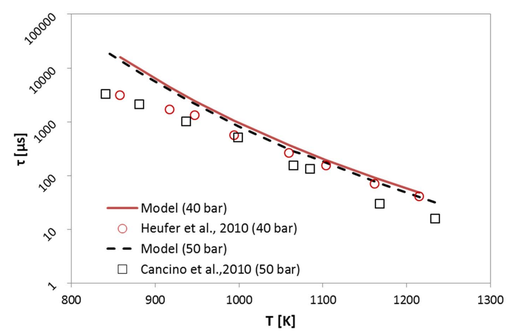

Fig 6. Ignition delay time of EtOH/O_2/N_2 at stoichiometric condition, measurements from [9-10].

Summary

The flow reactor results show that at stoichiometric and oxidizing conditions, oxidation is initiated at 725−750 K. For reducing conditions, the major consumption of oxygen happens at 775−800 K and with increasing temperature, concentrations of products of the reduction process (e.g. methane) increased monotonically.

The present model in general provides a satisfactory agreement with the measurements in the flow reactor. However, the model requires further improvement for prediction of ignition delay time at low temperatures and also for laminar burning velocity.

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