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Propane Oxidation at High Pressure and Intermediate Temperatures

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Experimental: Laminar Flow Reactor (FR)

- ❖ Quartz reactor to minimize surface reactions
- ❖ Steel pressure shell to achieve high pressures
- ❖ Temperature: 500–900 K
- ❖ Pressure: 100 bar
- ❖ Isothermal Zone Length: 42–44 cm
- ❖ Residence time: 8–11 s
- ❖ Measurement via GC and Gas Analyzer

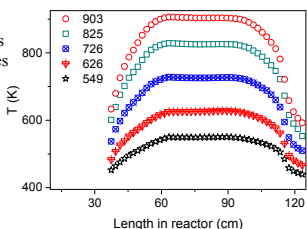


Fig 1. Temperature profile measured inside the pressure-shell wall of the reactor

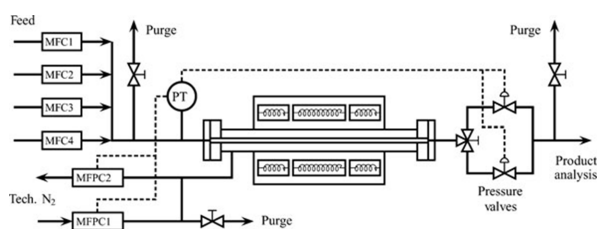


Fig 2. Schematic diagram of the high pressure laminar flow reactor

Chemical Kinetics Model

- ❖ H₂/CO/HC's subsets from recent work by Glarborg et al. [1–3].
- ❖ C₃ subset is reviewed and introduced in *p.w.*
- ❖ Low temperature sequences for propane oxidation is adopted from Goldsmith et al. [4].

Results: Flow Reactor (FR)

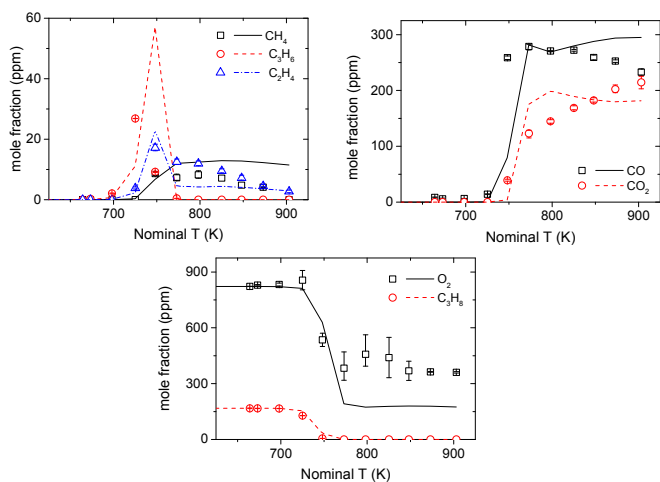


Fig 3. Experiments in the flow reactor at 100 bar pressure. The initial conditions were 168/ 822 ppm of C₃H₈/O₂ in N₂ (Φ=1). Residence time varies between 8 and 11 s.

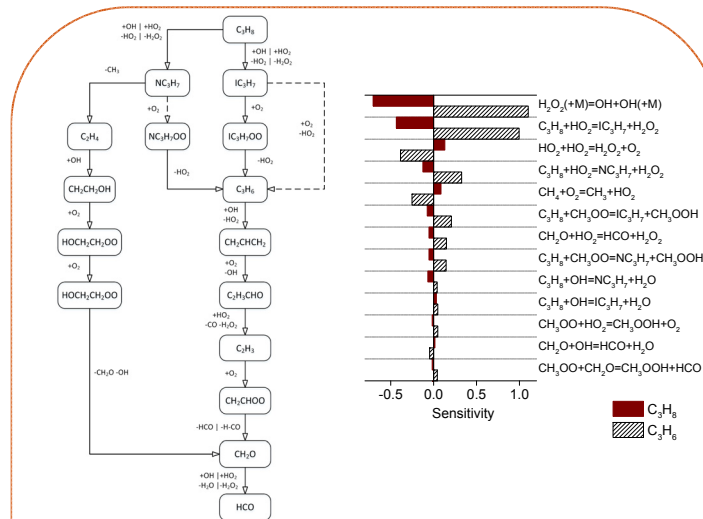


Fig 4. Left: Reaction pathways of propane oxidation at conditions investigated in the flow reactor (100 bar, 750 K). Right: Sensitivity of C₃H₈ and C₃H₆ prediction under flow-reactor conditions (100 bar, 750 K).

Results: Comparing the Model with Literature

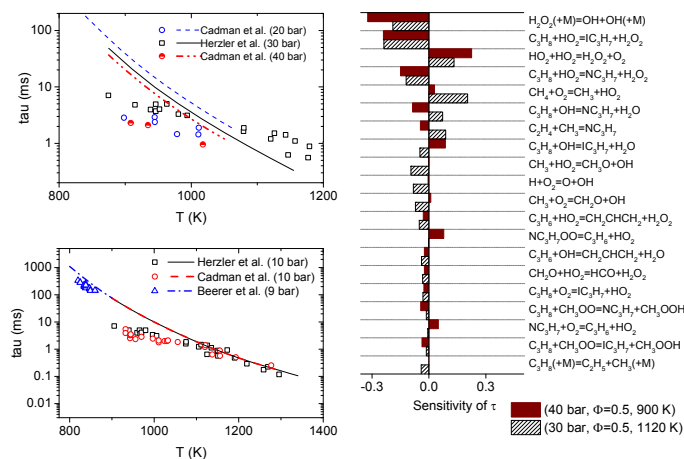


Fig 5. Left: Ignition delay times of propane. The experiments are from Herzler et al. [5] and Cadman et al. [6] (2.1% C₃H₈ + 20.6% O₂ in N₂, Φ=0.5), and Beerer et al. [7] (2.5% C₃H₈ + 20.5% O₂ in N₂, Φ=0.6). Right: Sensitivity of ignition delay time of propane to reaction rate constants (2.1% C₃H₈ + 20.6% O₂ in N₂, Φ=0.5).

Summary & Future Work

- ❖ Propane oxidation in the flow reactor:
 - Onset at 725–750 K (100 bar, Φ=1)
 - Accurate model prediction
 - Importance of abstraction reaction C₃H₈+ HO₂
- ❖ The model prediction of ignition delay times:
 - Over-prediction at intermediate T (900–1000 K)
 - Inaccuracy in transition from low-T to high-T regimes
- ❖ Further experiments on propane oxidation at different P and Φ are planned.
- ❖ Further work is required to improve the model prediction, especially for ignition delays.

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