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## Ignition of DME and DME/CH<sub>4</sub> at High Pressure: Flow Reactor Experiments and Kinetic Modeling

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## Abstract

The pyrolysis and oxidation of dimethyl ether (DME) and its mixtures with methane were investigated at high pressures (50 and 100 bar) and intermediate temperatures (450–900 K) in a laminar flow reactor. DME pyrolysis started at 825 K (at 50 bar). The onset of DME reaction was detected at 525–550 K (at 50 bar), independent of stoichiometry. The negative temperature coefficient (NTC) zone in the DME profile always included temperatures of 575–625 K. A profound promoting effect of DME addition on the ignition of methane was observed as the onset of reaction was shifted to lower temperatures by 50–150 K (at 100 bar).

## Objectives

- Study oxidation/pyrolysis of DME at intermediate temperatures (450–900 K) and high pressures (50–100 bar) in a laminar flow reactor
- Investigate the effect of adding DME on the oxidation of methane at intermediate temperatures and high pressures
- Investigate the effects of stoichiometry on DME and CH<sub>4</sub>/DME oxidation
- Develop a chemical kinetic model
- Evaluate the model against presented data as well as data from literature

## Experimental Setup: Laminar Flow Reactor

- Plug-flow conditions
- Quartz reactor to minimize the effects of heterogeneous reactions
- Temperature: 450–900 K
- Pressure: 50–100 bar
- Flow: 3.2–4.5 NL/min
- Residence time: 4–16 s
- GC measurements at the downstream

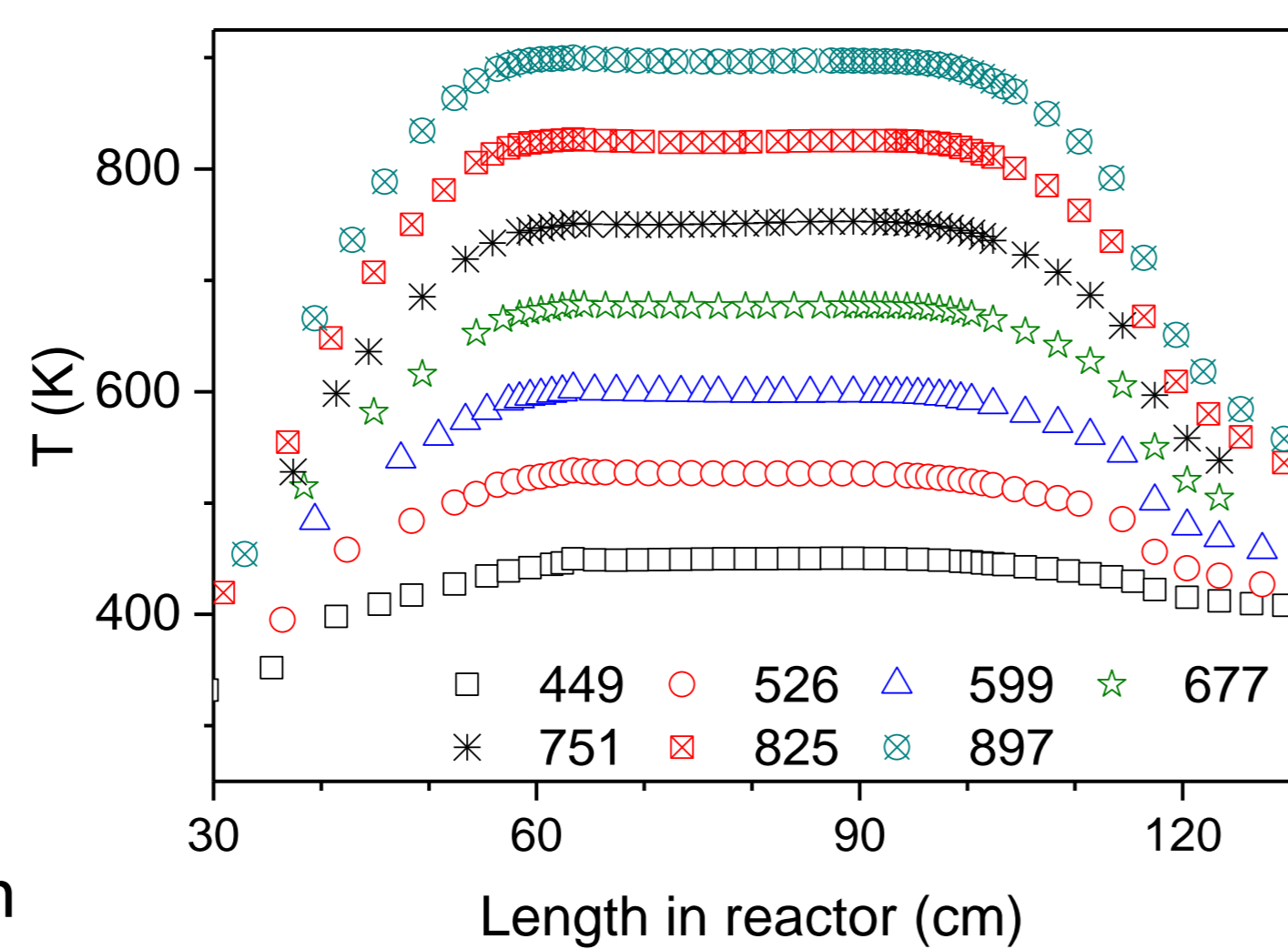


Figure 1: Measured temperature profiles across the reaction zone (4.53 NL/min of N<sub>2</sub> at 50 bar).

## Chemical Kinetic Model

- Founded on previous work from the same laboratory [1, 2]
- DME submodel from Zhao et al. [3]
- Formic acid submodel from Marshall and Glarborg [4]
- Methylformate subset from Dooley et al. [5]

## Results

- DME pyrolysis: 825 K
- DME oxidation: 525 K (independent of  $\Phi$ )
- NTC zone: including 575–625 K (a function of  $\Phi$ )

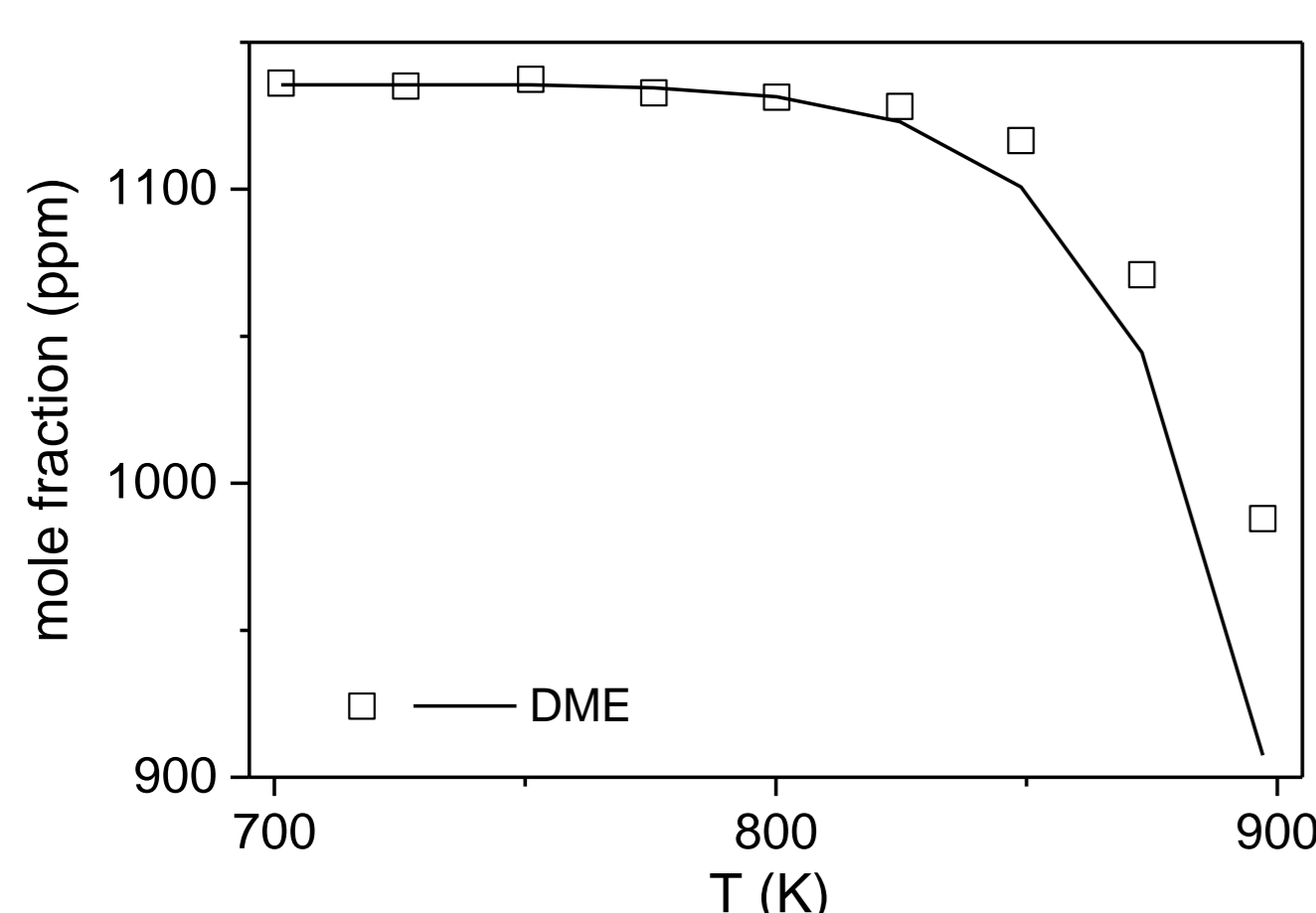


Figure 2: Pyrolysis of DME at 50 bar (1136 ppm DME in N<sub>2</sub>).

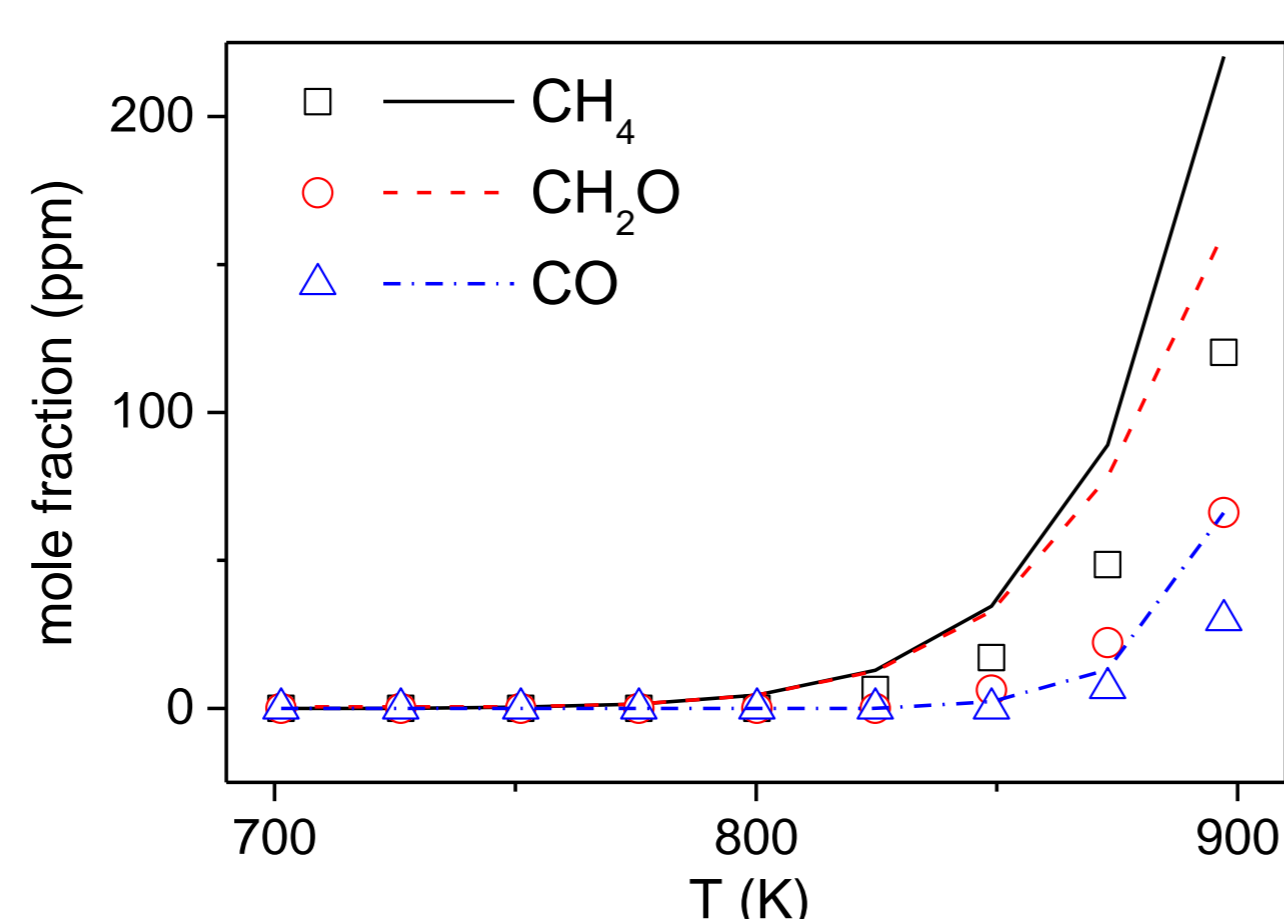


Figure 3: Pyrolysis of DME at 50 bar (1136 ppm DME in N<sub>2</sub>).

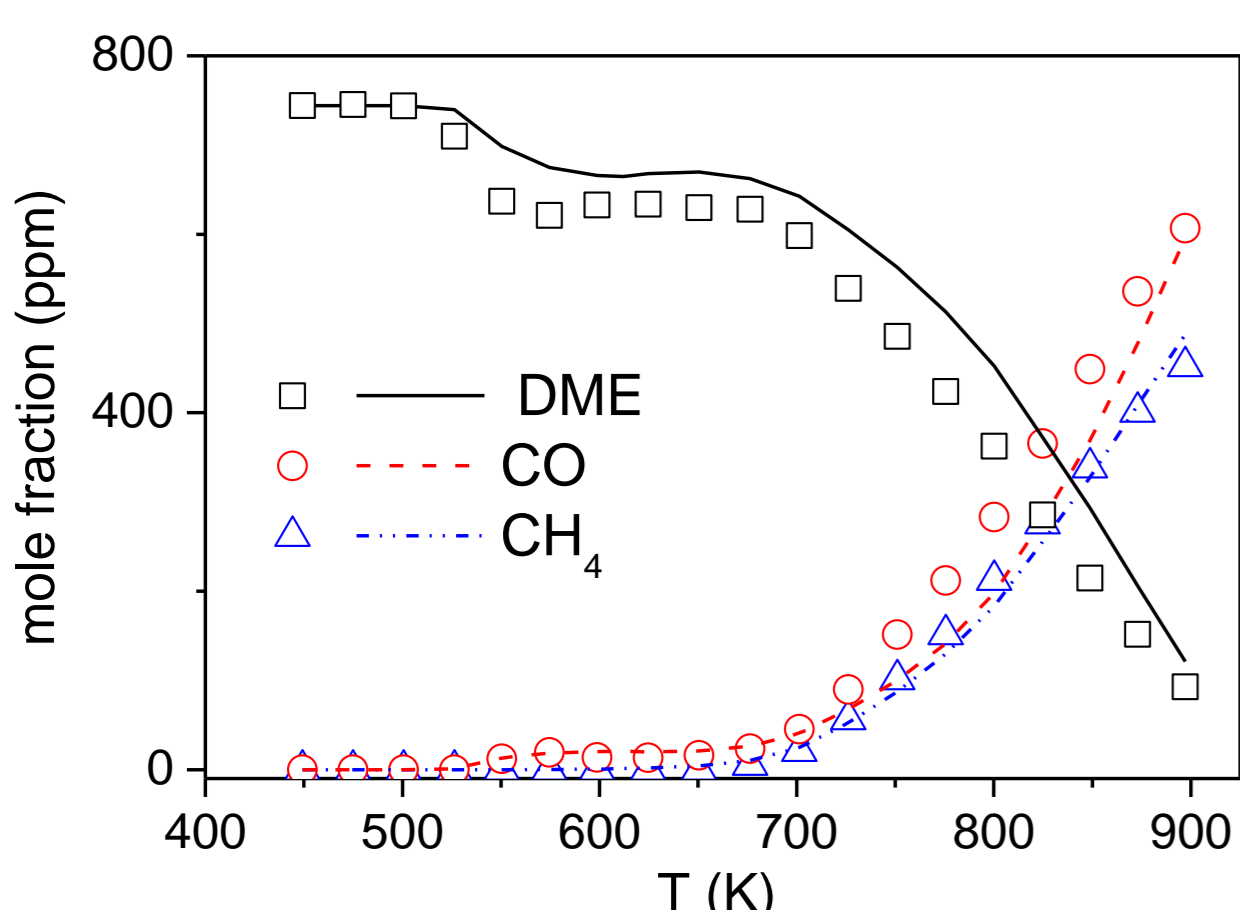


Figure 4: DME oxidation under fuel-rich conditions ( $\Phi=20$ , 744 ppm DME) at 50 bar.

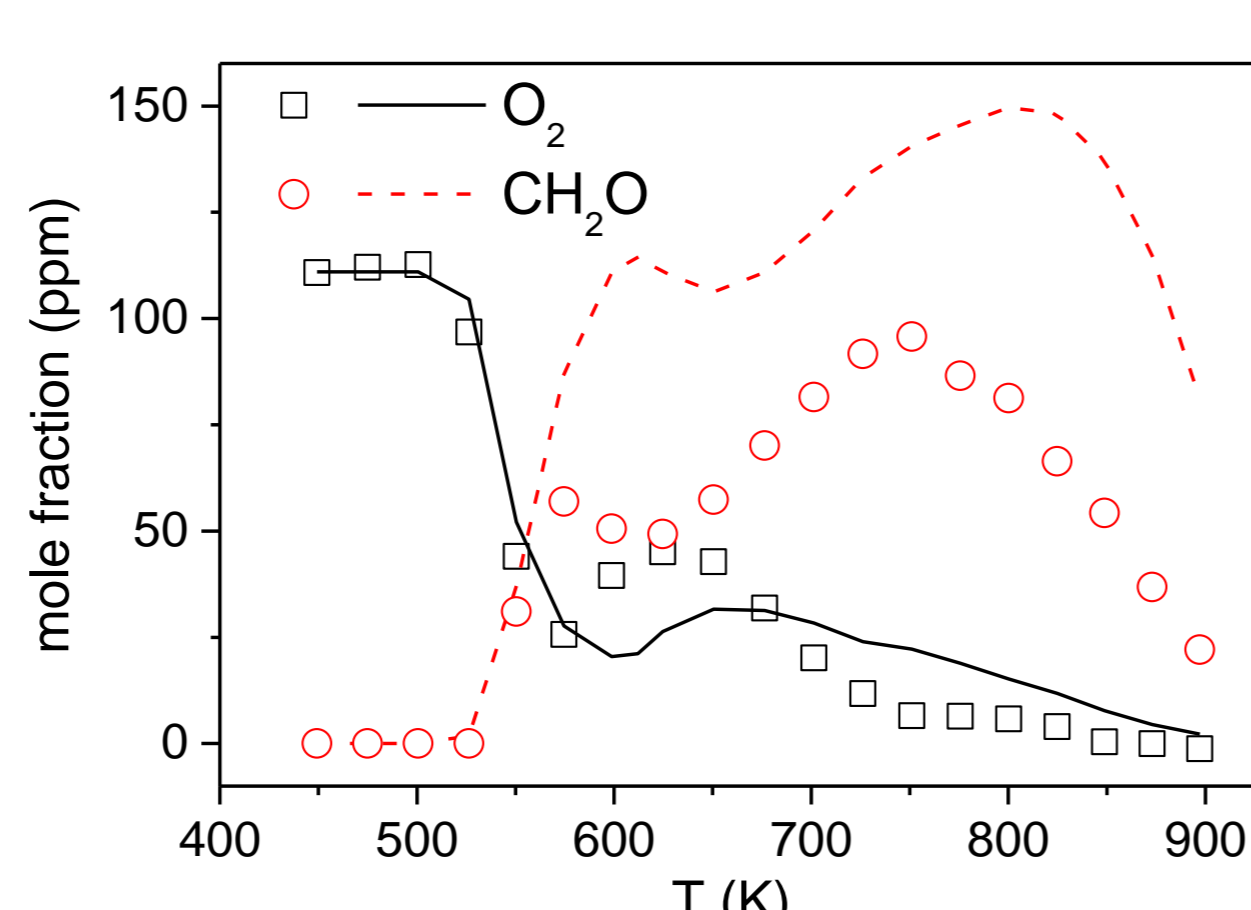


Figure 5: DME oxidation under fuel-rich conditions ( $\Phi=20$ , 744 ppm DME) at 50 bar.

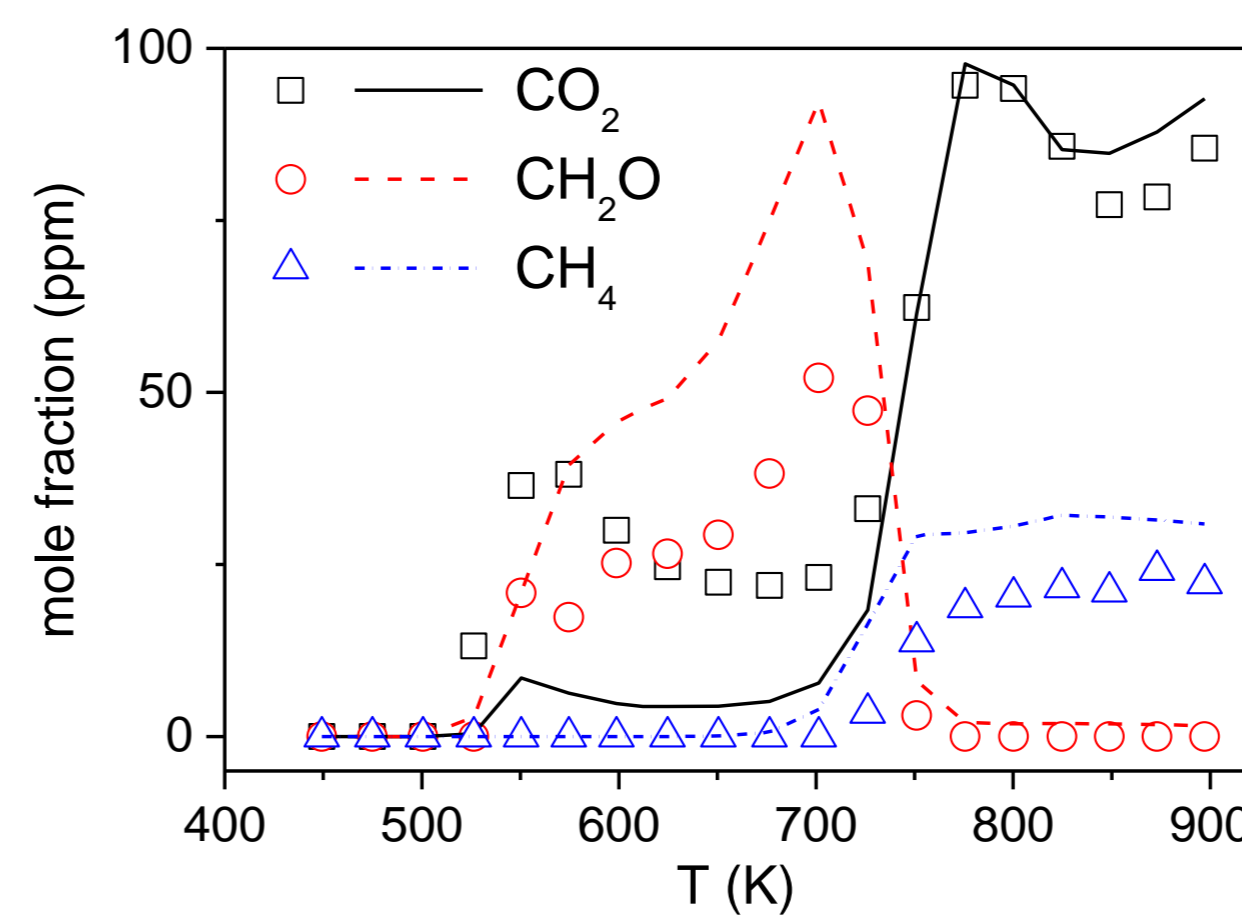


Figure 6: DME oxidation under stoichiometric conditions ( $\Phi=1$ , 268 ppm DME) at 50 bar.

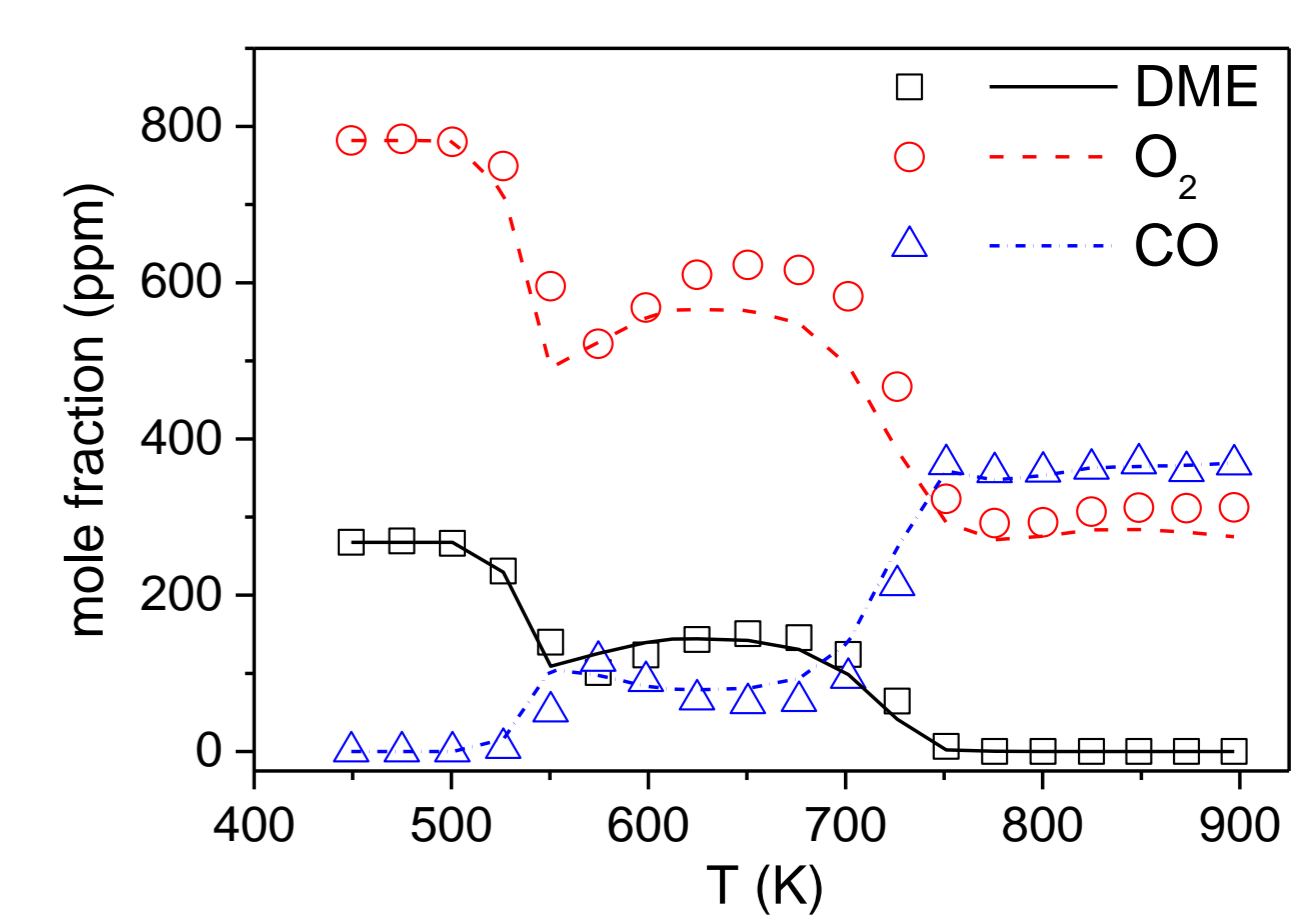


Figure 7: DME oxidation under stoichiometric conditions ( $\Phi=1$ , 268 ppm DME) at 50 bar.

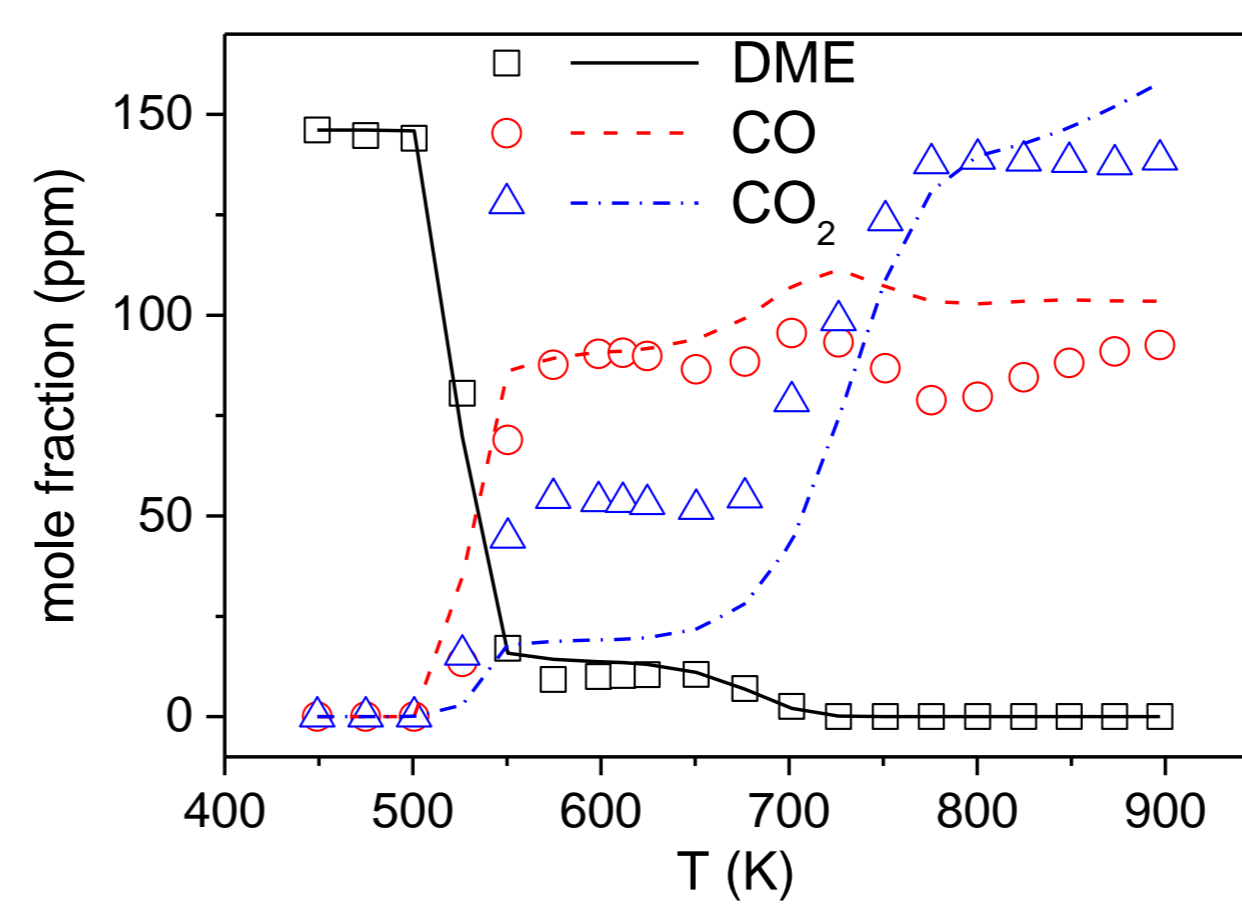


Figure 8: DME oxidation under fuel-lean conditions ( $\Phi=0.04$ , 146 ppm DME) at 50 bar.

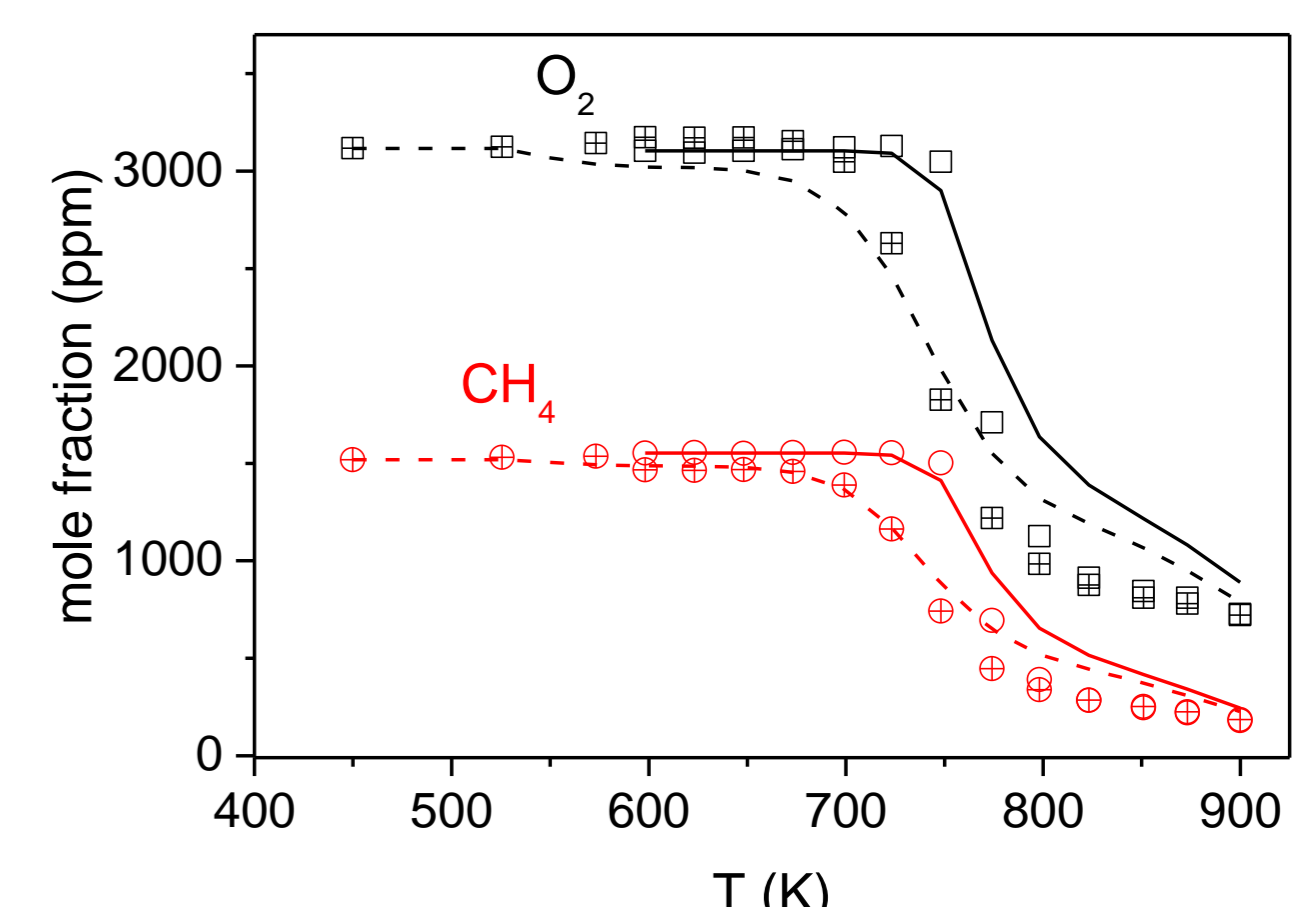


Figure 9: DME addition to methane under stoichiometric conditions ( $\Phi=1$ , 100 bar). Open symbols/solid lines: the neat CH<sub>4</sub> experiment; Crossed symbols/dashed lines: DME/CH<sub>4</sub>=3.2% (48 ppm of DME)

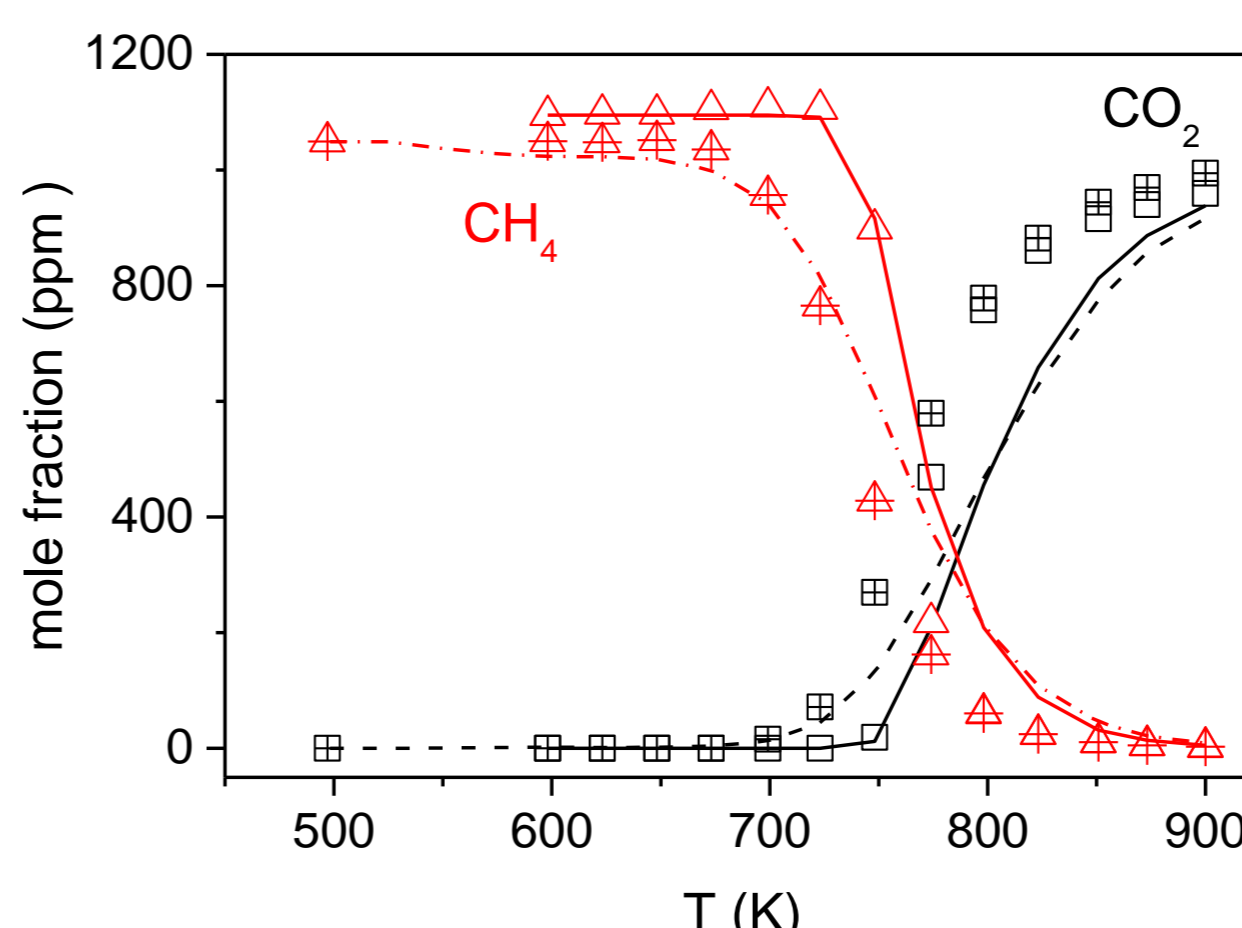


Figure 10: DME addition to methane under fuel-lean conditions ( $\Phi=0.06$ , 100 bar). Open symbols/solid lines: the neat CH<sub>4</sub> experiment; Crossed symbols/dashed lines: DME/CH<sub>4</sub>=3.6% (38 ppm of DME)

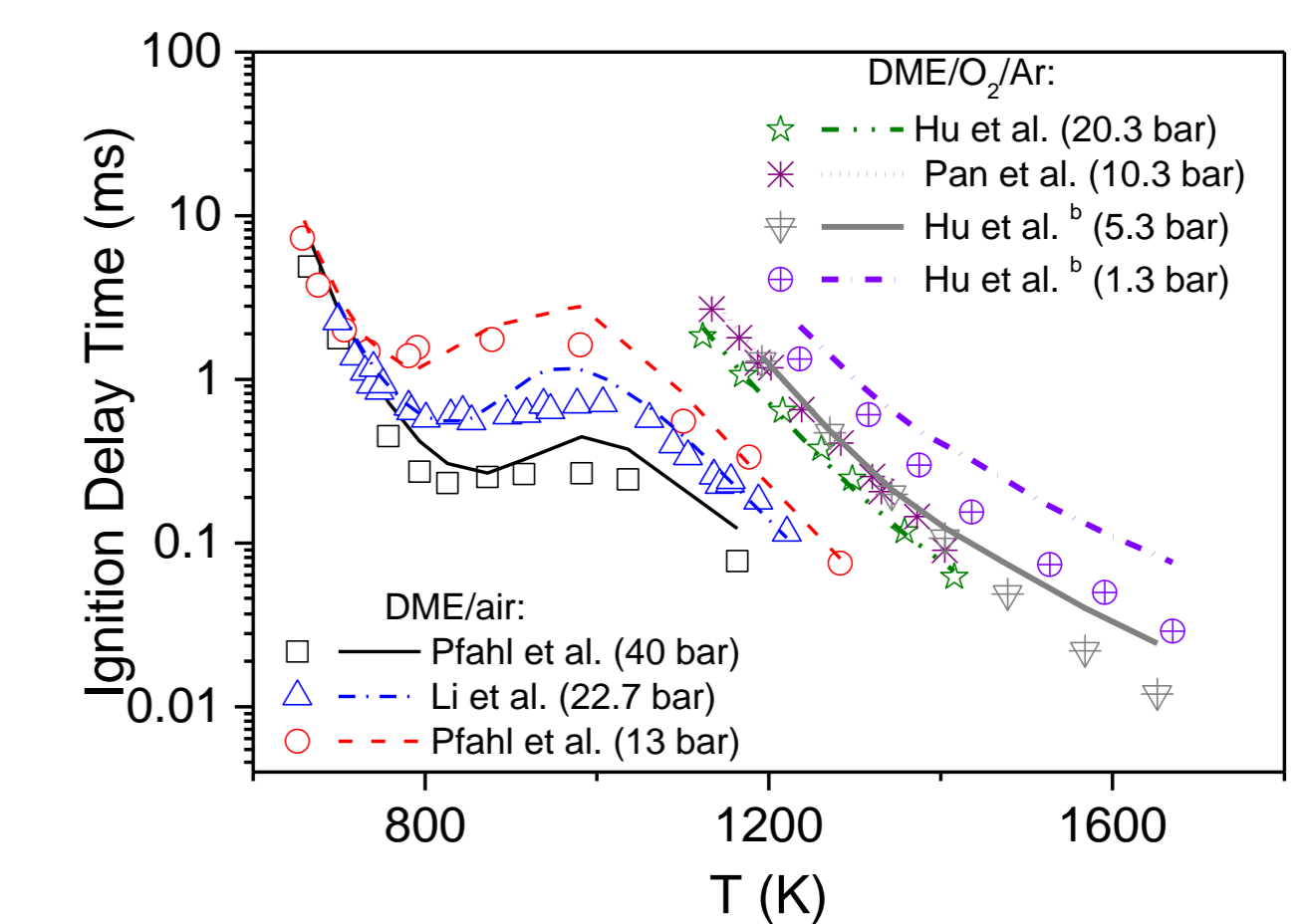


Figure 11: Ignition delay times of stoichiometric DME/air (data from Pfahl et al. and Li et al.) and DME/O<sub>2</sub>/Ar (data from Hu et al., Pan et al., Hu et al.<sup>b</sup>). Lines denote the prediction of the present model assuming constant  $u$  &  $v$ .

## Conclusions

The pyrolysis and oxidation of DME and its effect on methane oxidation as an additive have been investigated in a flow reactor at high pressures and intermediate temperatures. It was found that DME pyrolysis started around 825 K at 50 bar pressure. The DME oxidation experiments at 50 bar gave the onset temperature of reaction at 525 K, independent of  $\Phi$ . Further experiments at 100 bar showed that by adding a small amount of DME to methane its ignition could effectively be accelerated. A model developed for DME/CH<sub>4</sub> oxidation was evaluated over a wide range of pressure, temperature, and stoichiometries. The model generally compared well with the data from the flow reactor. Further work is needed to focus on interaction between DME and CH<sub>4</sub> in the model to address the premature DME depletion in CH<sub>4</sub>/DME mixtures. The presented data extended the experimental benchmark for oxidation at high pressures and intermediate temperatures. Such benchmark are vital in validating chemical kinetic models developed for addressing problems in real conditions.

## References

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