Experimental and kinetic modeling study of laminar coflow diffusion methane flames doped with *iso*-butanol

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1. External validations

1.1 Flow tube pyrolysis of iso-butanol

Flow tube pyrolysis of iso-butanol under 30 and 760 Torr reported in the work of Cai et al. [1] was adopted to validate the fuel decomposition sub-mechanism. The composition of the inlet gas flow was 3% of iso-butanol and 97% of Argon. Kinetic modeling under these conditions was performed by plug flow reactor code in OpenSMOKE [2]. The results are presented in Figs. S1-S3.

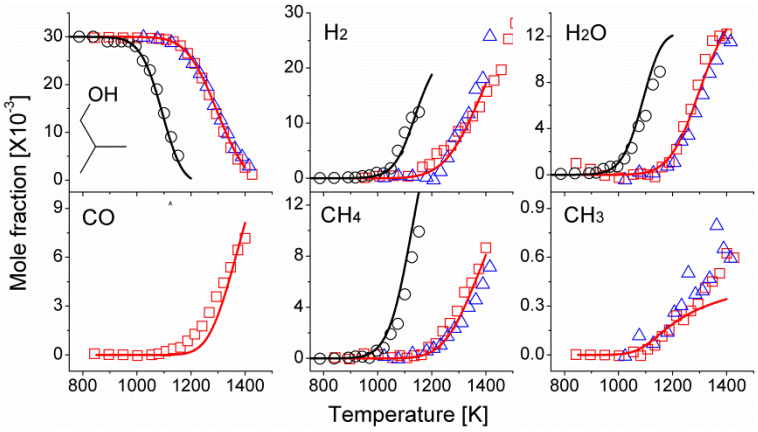

Figure S1 Model predictions (lines) and experimental data (symbols) of the reactant and major products in the pyrolysis of iso-butanol. The black circle indicates the experimental data in 760 Torr, blue triangle and red square indicate those in 30 Torr.

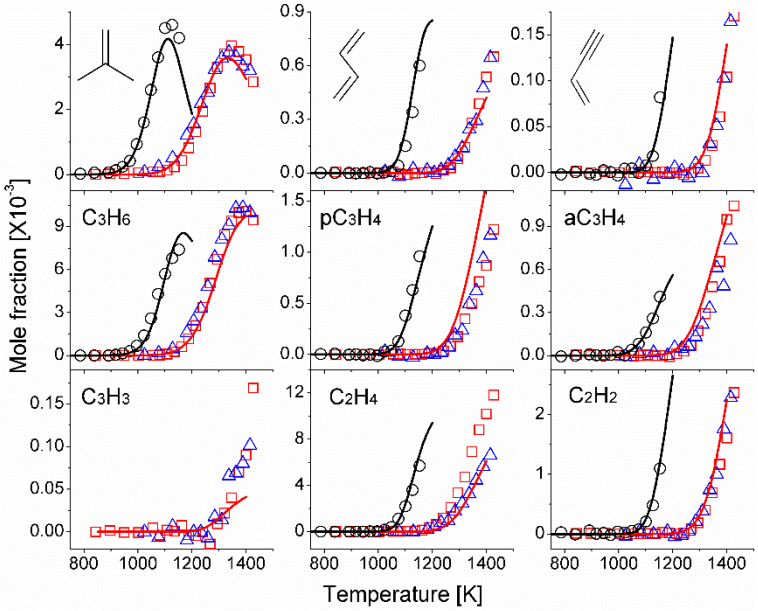

Figure S2 Model predictions (lines) and experimental data (symbols) of the hydrocarbon intermediates. The black circle indicates the experimental data in 760 Torr, blue triangle and red square indicate those in 30 Torr.

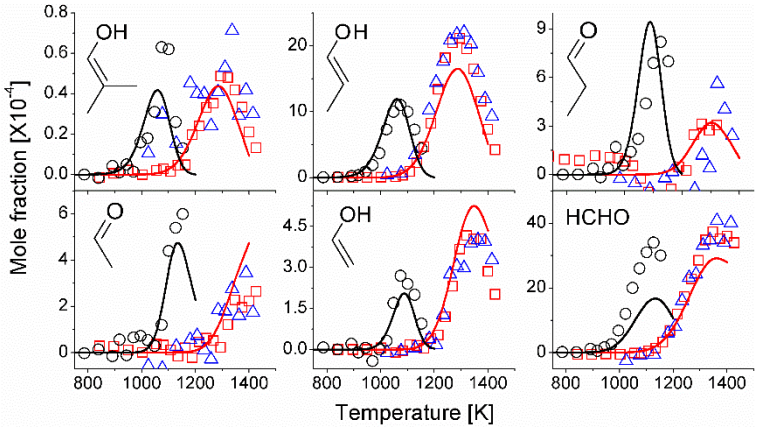

Figure S3 Model predictions (lines) and experimental data (symbols) of the oxygenated intermediates. The black circle indicates the experimental data in 760 Torr, blue triangle and red square indicate those in 30 Torr.

1.2 Pyrolysis of iso-butanol in shock tube

Shock tube pyrolysis of iso-butanol performed by Stranic et al. [3] was also validated to the present model. The time history of OH, H_2O, CO and CH_4 reported in their work was well reproduced, as shown in Fig. S5. It was also modeled by OpenSMOKE [2].

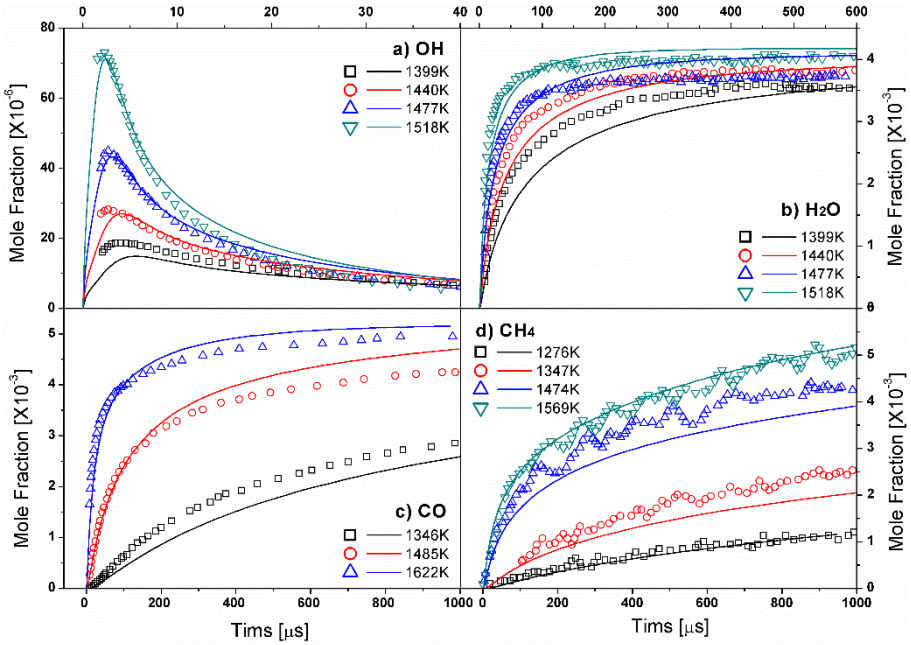

Figure S4 Model predictions (lines) and experimental data (symbols) of shock tube iso-butanol pyrolysis.

1.3 Oxidation of iso-butanol in jet-stirred reactor

Togbé et al. [4] investigated the oxidation of iso-butanol in an equivalence ratio range of 0.5 - 4.0 under the pressure of 10 atm in a jet-stirred reactor. Reactants as well as the intermediates were measured by gas chromatography. The model predictions of the experimental data are shown in Fig. S5-S8.

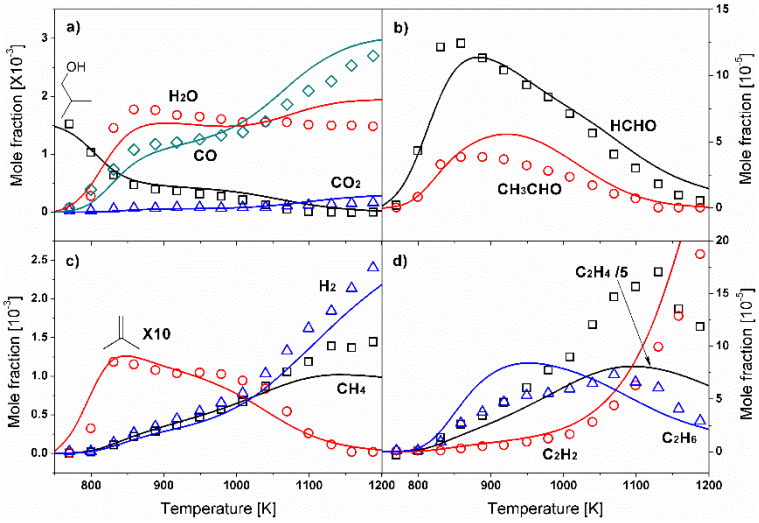

Figure S5 Model predictions of iso-butanol oxidation at ϕ = 4.0.

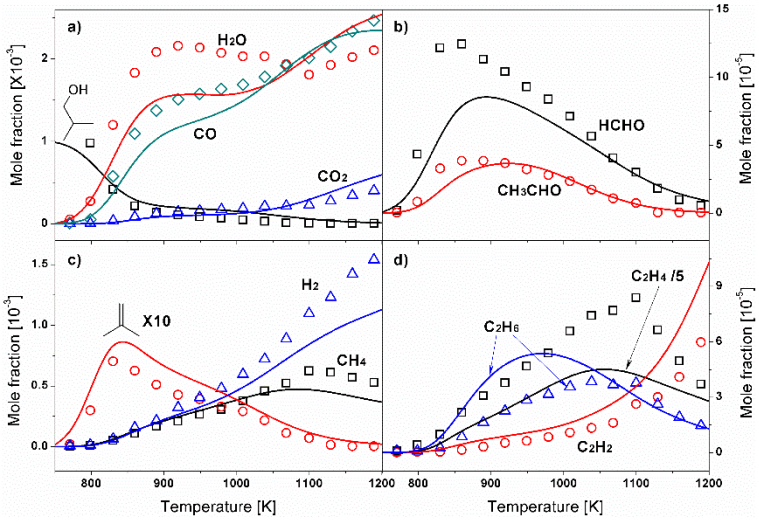

Figure S6 Model predictions of iso-butanol oxidation at ϕ = 4.0.

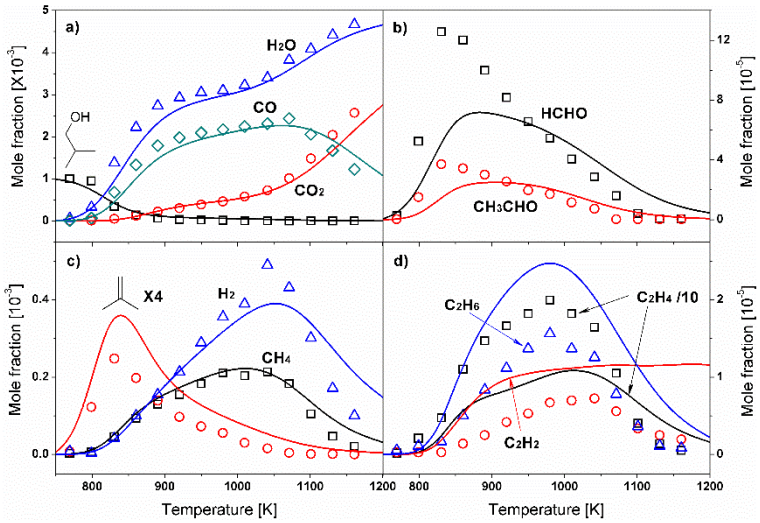

Figure S7 Model predictions of iso-butanol oxidation at ϕ = 4.0.

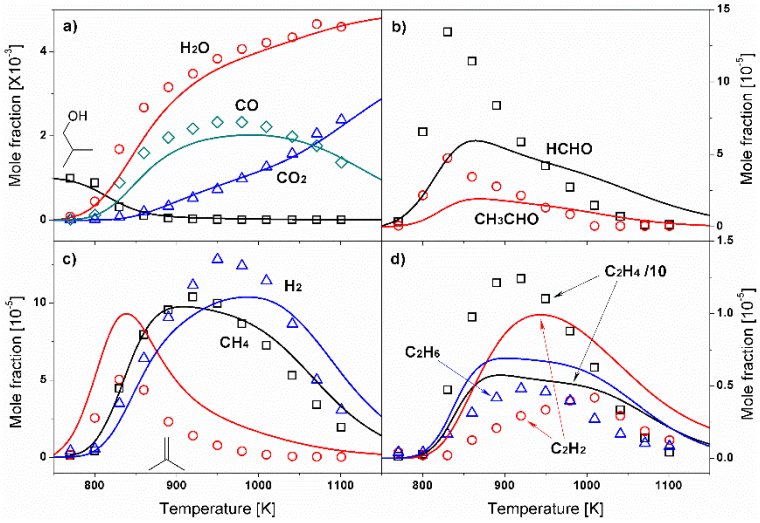

Figure S8 Model predictions of iso-butanol oxidation at ϕ = 4.0.

1.4 Premixed flat flame of iso-butanol

Hansen et al. [5] diagnosed the low-pressure premixed rich flame with the help of SVUV-PIMS method. Their experimental data reported in [5] was adopted for the validation of the present model. The comparison of modeling and experimental results are presented in Fig. S9.

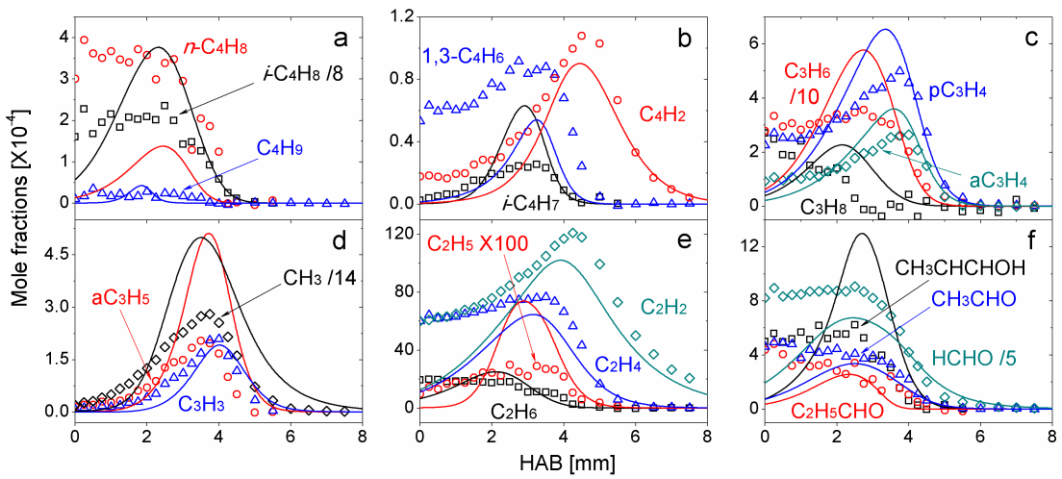

Figure S9 Model predictions of Premixed flat flame of iso-butanol at ϕ = 1.5.

1.5 Counter flow diffusion flame of iso-butanol

Counter flow diffusion flame is another kind of diffusion flame that can be modeled as an approximated 1D flame. The performance of the model in this kind of flame reflects the accuracy and time consuming in the simulation of coflow diffusion flames. Grana et al. [6] sampled the counter flow diffusion flame with a quartz probe and quantified the concentrations of flame species by gas chromatography. The flame condition is 100 s^{-1} in strain rate under 1 atm. The temperature of the inlet fuel mixture and oxidizer is 353 and 298 K. Laminar flame model in OpenSMOKE was used to simulation this flame, and the results are presented in Fig. S10.

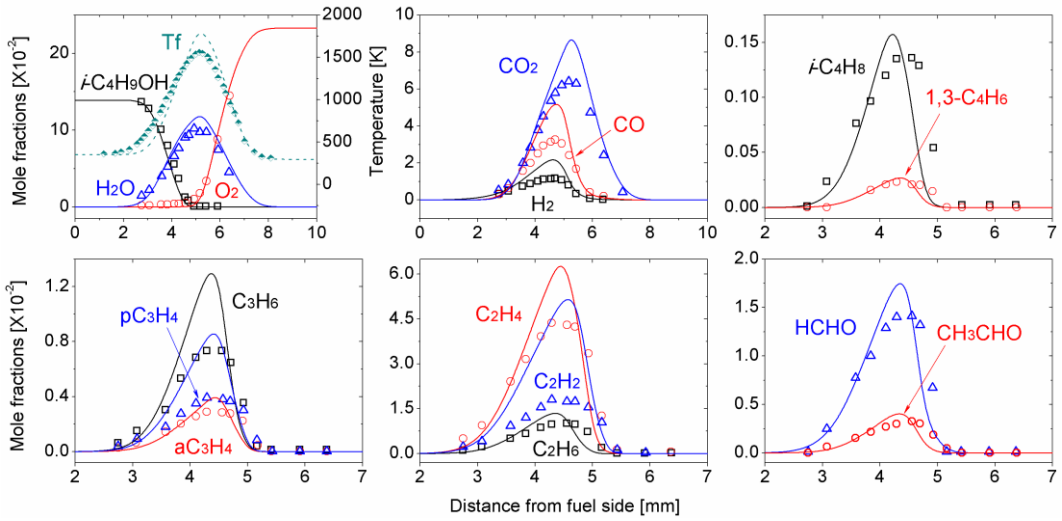

Figure S10 Model predictions of counter flow diffusion flame of iso-butanol.

References

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