

## *Supplemental Material for*

### **Experimental and Updated Kinetic Modeling Study of Neopentane Low Temperature Oxidation**

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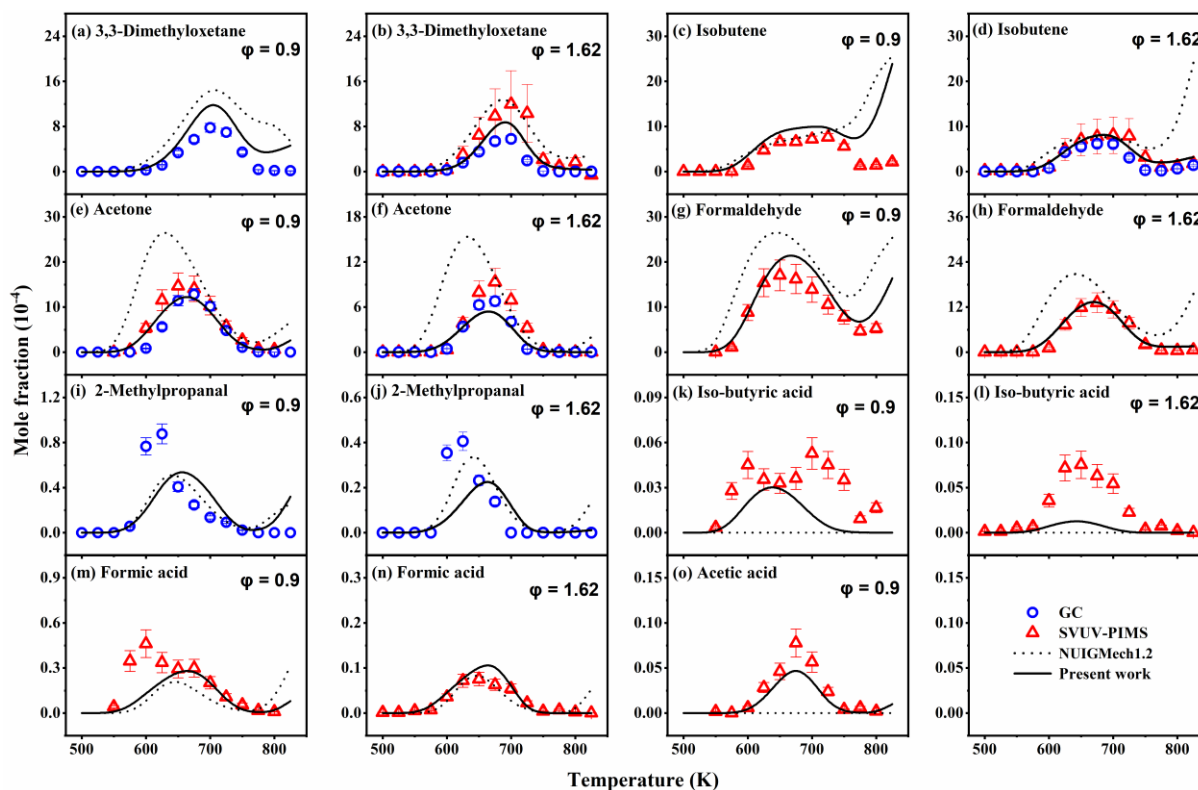
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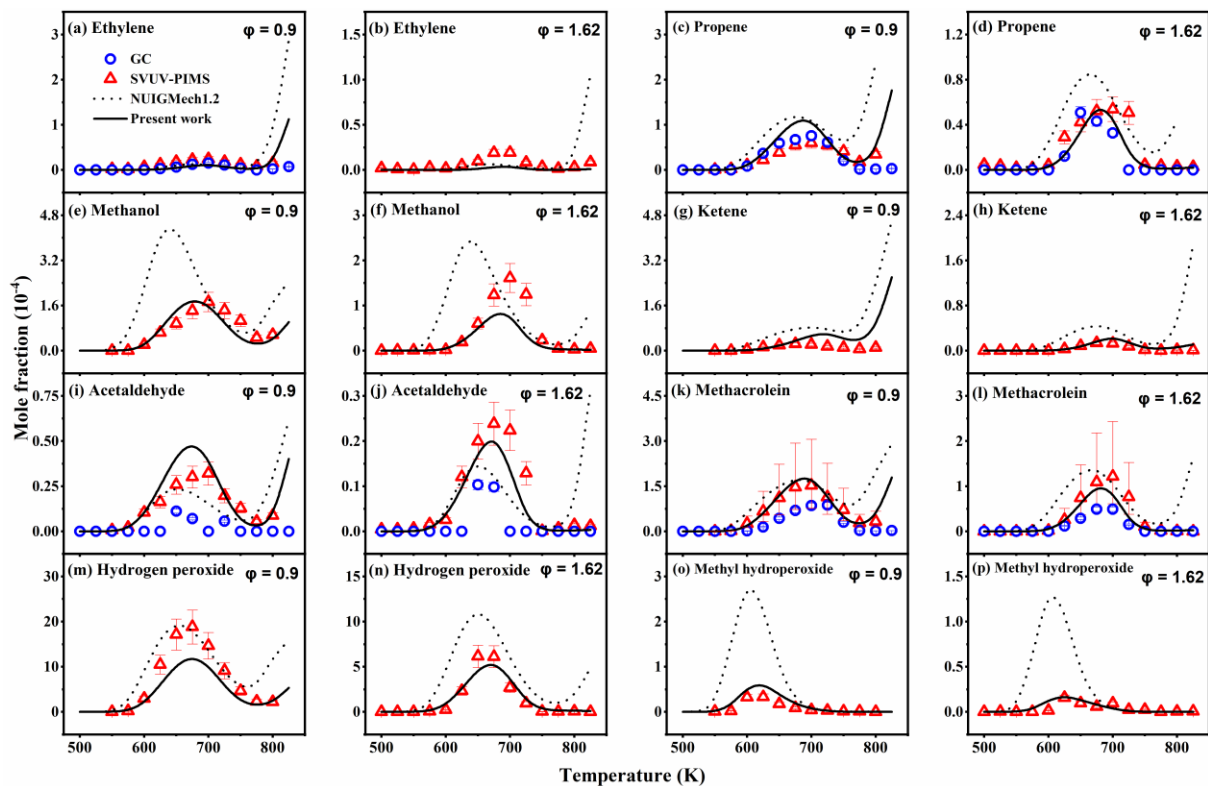
## Section 1: Model validation against speciation data measured in this work

### S1.1 Low temperature experiment data

**Figure S1.** Measured (symbols) and model-predicted (lines) mole fraction profiles of 3,3-dimethyloxetane, isobutene, acetone, formaldehyde, 2-methylpropanal, iso-butyric acid, formic acid, and acetic acid at  $\phi = 0.9$  and  $\phi = 1.62$ . At  $\phi = 1.62$ , the formation of acetic acid was not detected by SVUV-PIMS. Dotted and solid lines represent the predicted results from the NUIGMech1.2,<sup>1</sup> and the present model, respectively. The error bar for the experimental data is given.

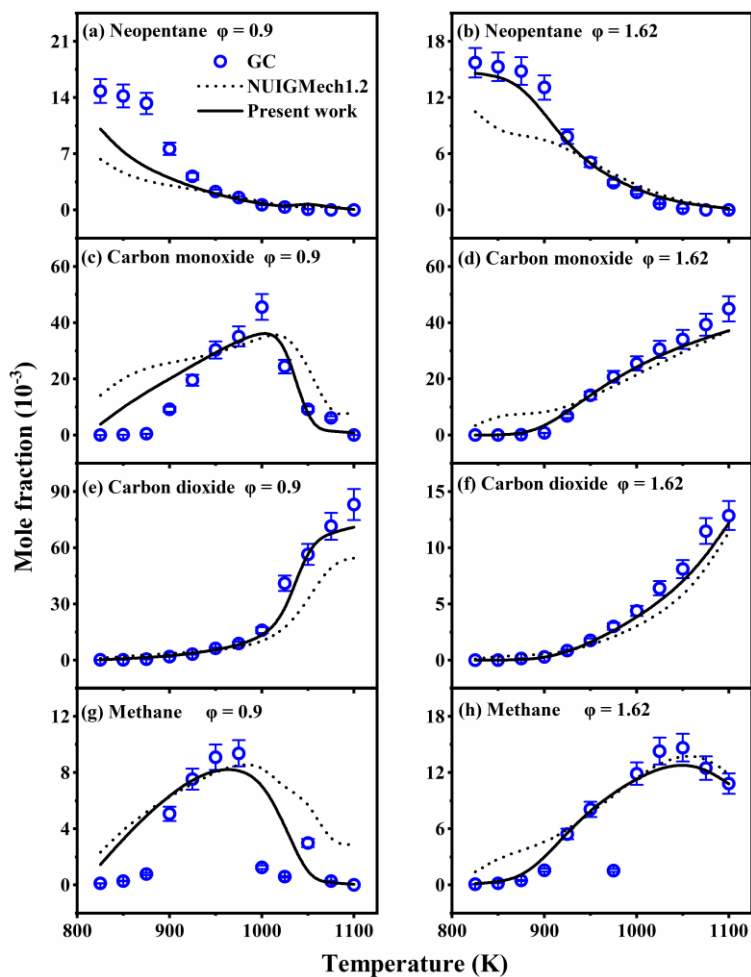


**Figure S2.** Measured (symbols) and model-predicted (lines) mole fraction profiles of ethylene, propene, methanol, ketene, acetaldehyde, methacrolein, hydrogen peroxide, and methyl hydroperoxide at  $\phi = 0.9$  and  $\phi = 1.62$ . Dotted and solid lines represent the predicted results by the NUIGMech1.2,<sup>1</sup> and the present model, respectively. The error bar for the experimental data is given.

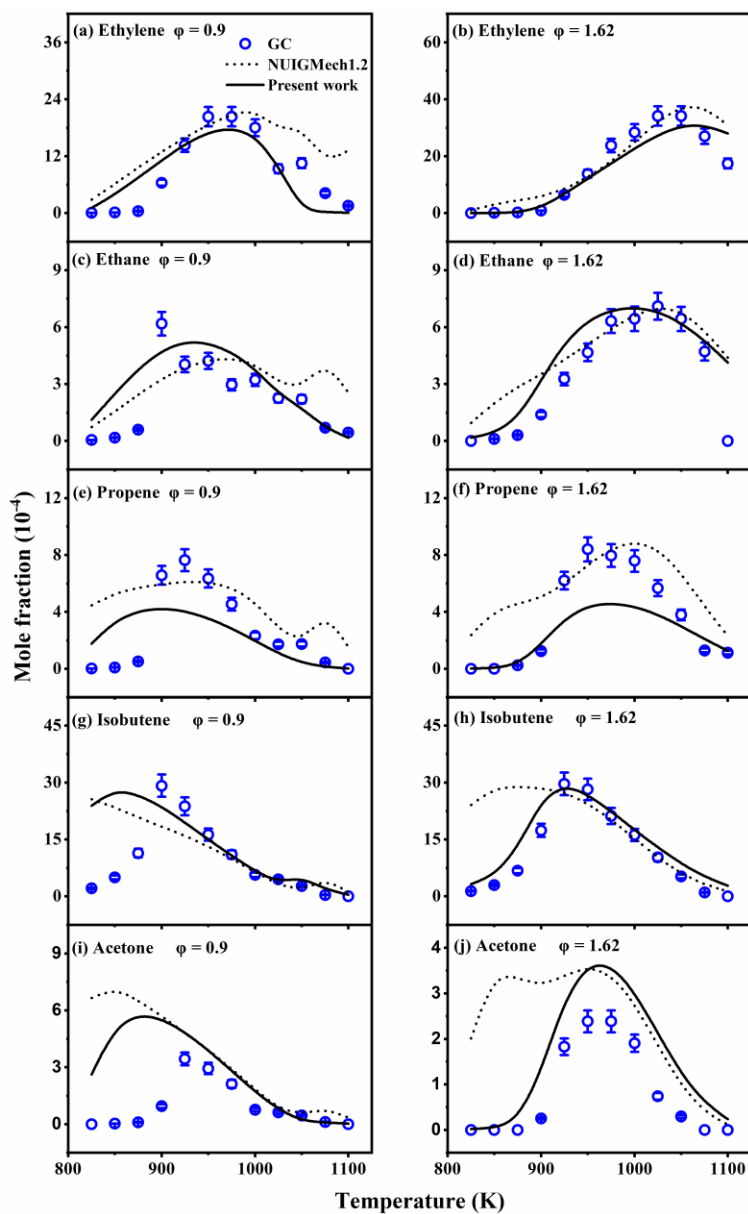


## S1.2 High temperature experimental data

**Figure S3.** Measured (symbols) and model-predicted (lines) mole fraction profiles of neopentane, carbon monoxide, carbon dioxide and methane at  $\phi = 0.9$  and  $\phi = 1.62$ . Dotted and solid lines represent the predicted results by the NUIGMech1.2,<sup>1</sup> and the present model, respectively. The error bar for the experimental data is given.

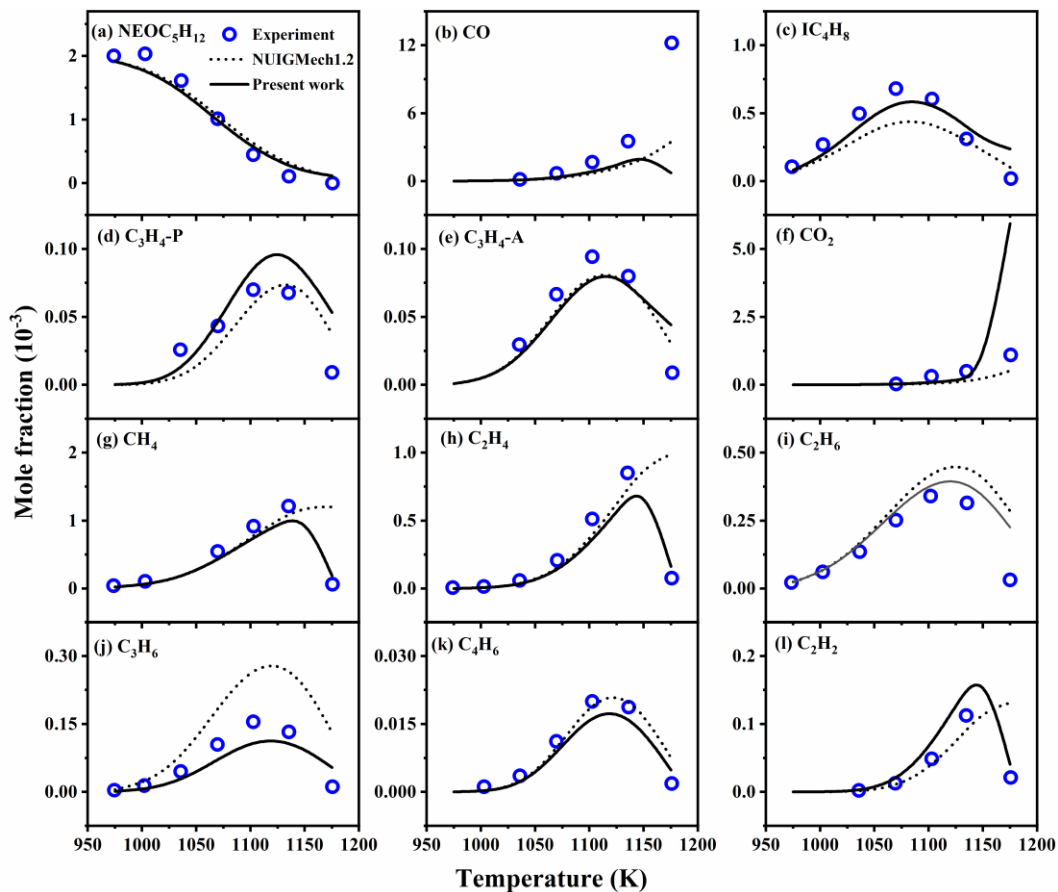


**Figure S4.** Measured (symbols) and model-predicted (lines) mole fraction profiles of ethylene, ethane, propene, isobutene, and acetone at  $\phi = 0.9$  and  $\phi = 1.62$ . Dotted and solid lines represent the predicted results by the NUIGMech1.2,<sup>1</sup> and the present model, respectively. The error bar for the experimental data is given.

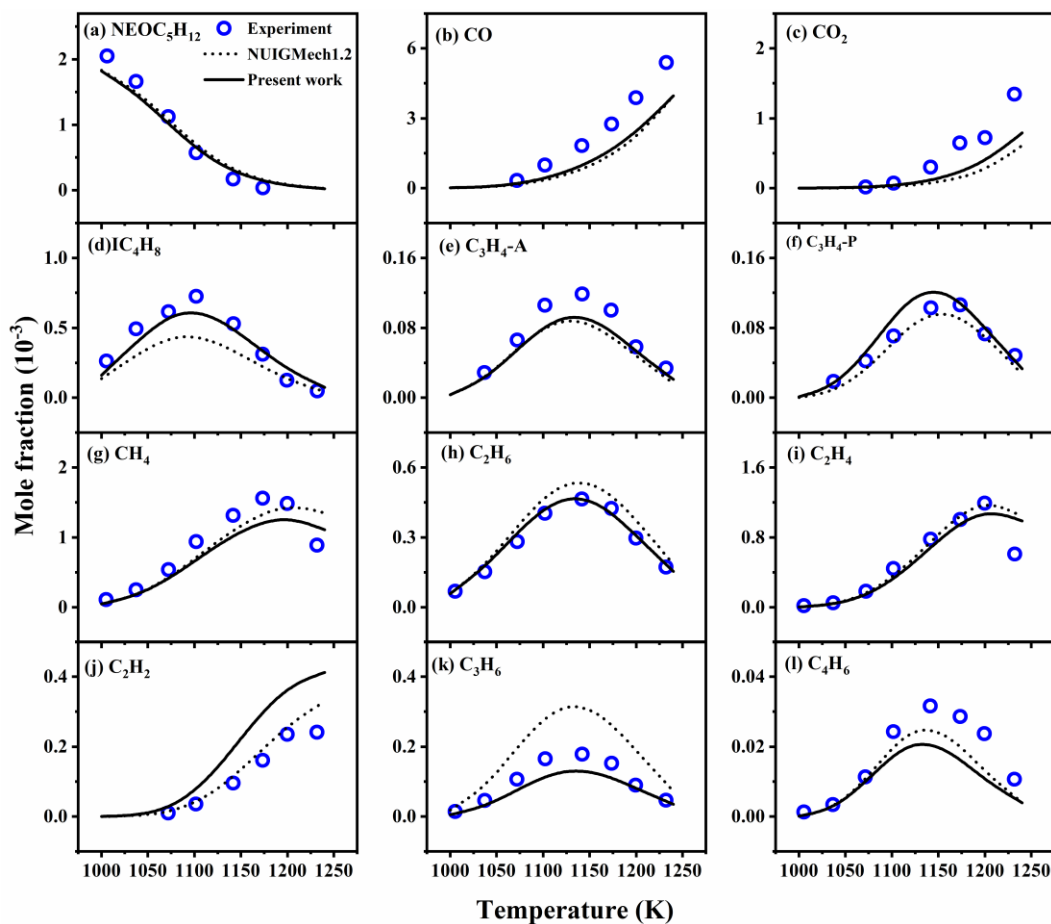


## Section 2: Model validation against speciation data reported in this literature

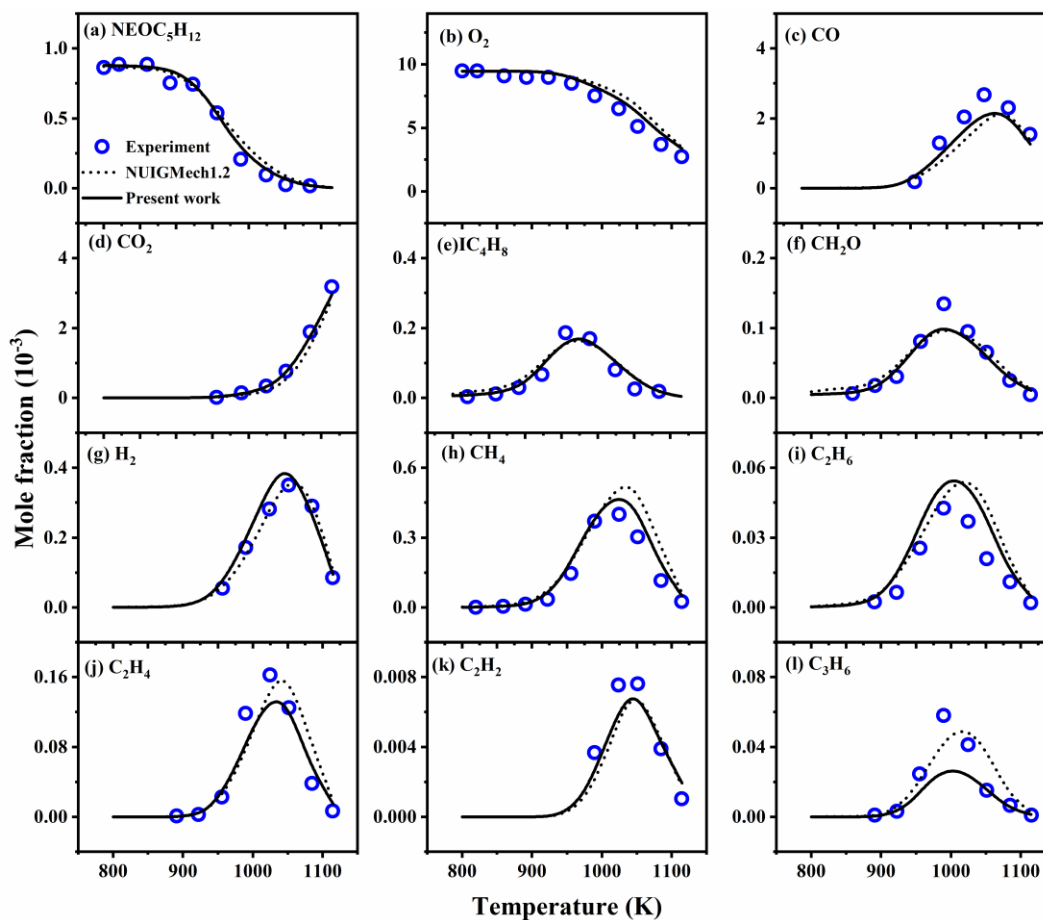
**Figure S5.** Measured (symbols) and model-predicted (lines) mole fraction profiles of neopentane and neopentane oxidation products at 1 atm. Experimental data are taken from Dagaut et al.<sup>2</sup> The experiment conditions were neopentane 0.2%, O<sub>2</sub>, 1.6%, N<sub>2</sub>, 98.2%;  $\tau = 0.2$  sec;  $\phi = 1$ . Dotted and solid lines represent the predicted results by the NUIGMech1.2,<sup>1</sup> and the present model, respectively.



**Figure S6.** Measured (symbols) and model-predicted (lines) mole fraction profiles of neopentane and neopentane oxidation products at 1 atm. Experimental data are taken from Dagaut et al.<sup>2</sup> The experiment conditions were neopentane 0.2%, O<sub>2</sub>, 0.8%, N<sub>2</sub>, 99%;  $\tau = 0.2$  sec;  $\phi = 2$ . Dotted and solid lines represent the predicted results by the NUIGMech1.2,<sup>1</sup> and the present model, respectively.



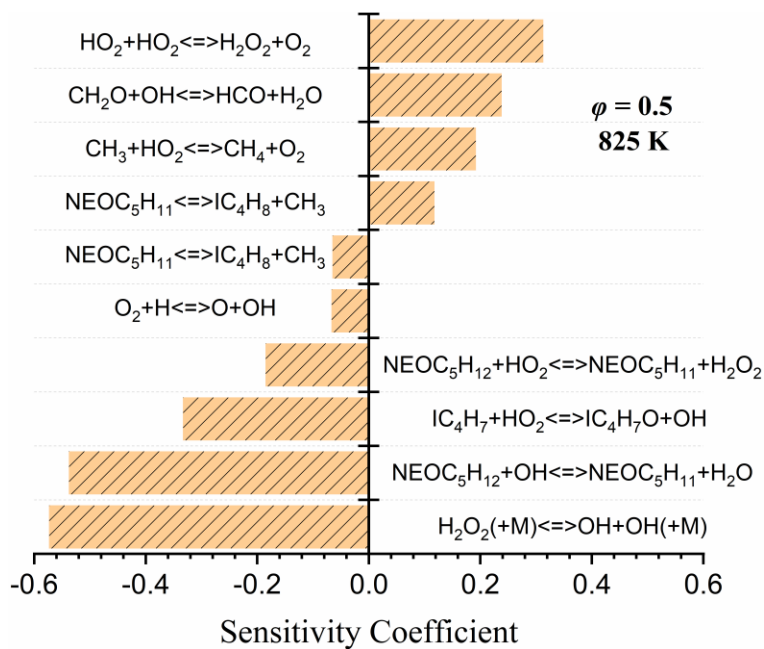
**Figure S7.** Measured (symbols) and model-predicted (lines) mole fraction profiles of neopentane and neopentane oxidation products at 10 atm. Experimental data are taken from Dagaut et al.<sup>2</sup> The experiment conditions were neopentane 0.1%, O<sub>2</sub>, 0.8%, N<sub>2</sub>, 98.2%;  $\tau = 2$  sec;  $\phi = 1$ . Dotted and solid lines represent the predicted results by the NUIGMech1.2,<sup>1</sup> and the present model, respectively.





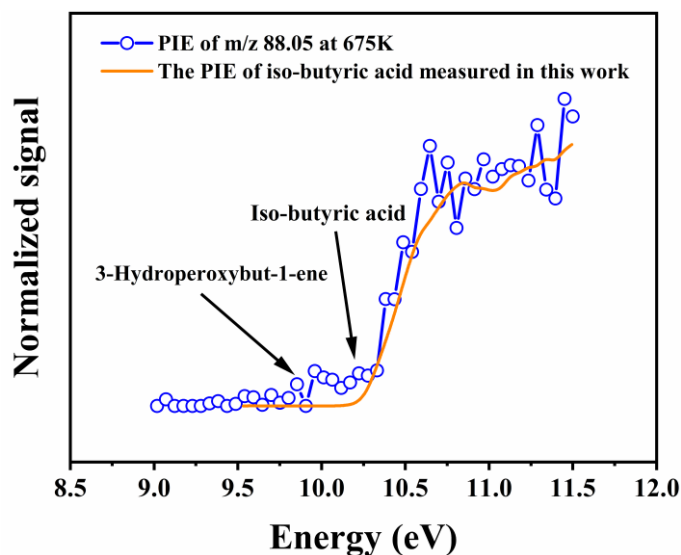
### Section 3: Sensitivity analyses based on the present model

Figure S8. Sensitivity analysis of the present model for neopentane at 825 K and  $\varphi = 0.5$ .

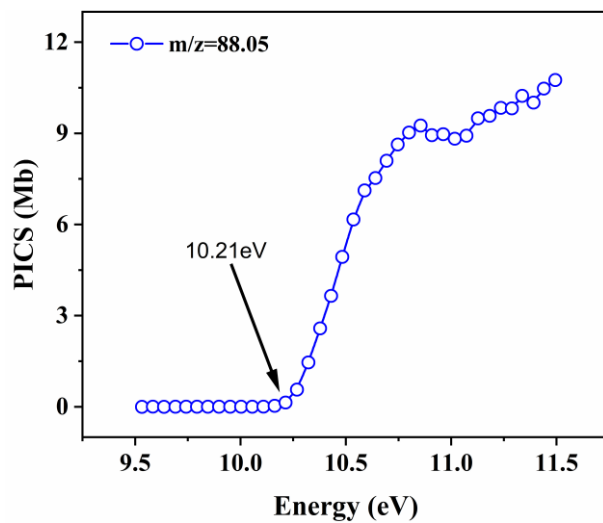


## Section 4: The identification of iso-butyric acid

**Figure S9.** The PIE of  $m/z$  88.05 registered in SVUV-PIMS at 675 K and  $\phi = 0.9$  (dots) compared to the PIE of iso-butyric acid measured in this work (orange line).



**Figure S10.** Absolute photoionization cross-section (PICS) of iso-butyric acid ( $m/z = 88.05$ ) measured in this work.

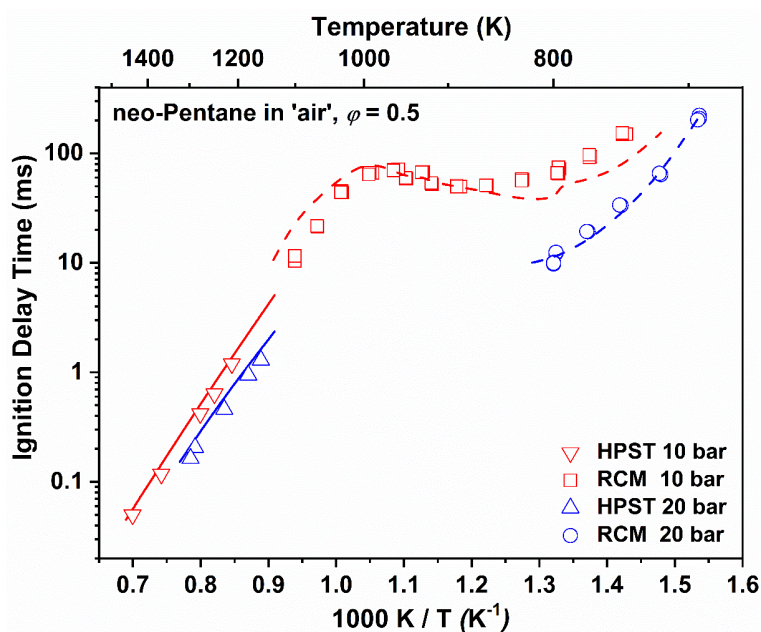


**Table S1.** Absolute PICS (Mb) of iso-butyric acid ( $m/z = 88.05$ ) measured in this work.

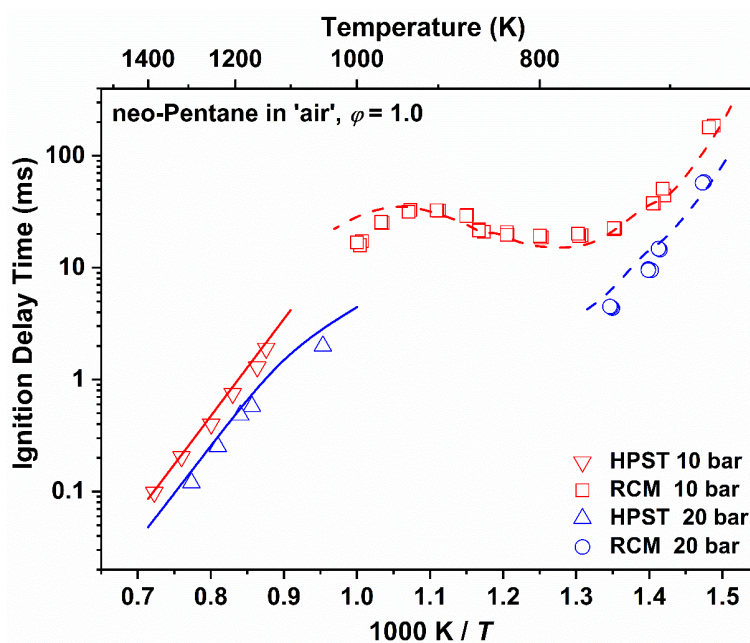
<b>Energy(eV)</b>	<b>PICS (Mb) m/z=88.05</b>	<b>Energy(eV)</b>	<b>PICS (Mb) m/z=88.05</b>
9.532	0	10.536	6.16679
9.584	0.00558	10.589	7.12261
9.637	0	10.64	7.53038
9.691	0.00123	10.693	8.09794
9.742	0.00141	10.746	8.63433
9.794	0.00125	10.8	9.02762
9.845	0.001	10.855	9.25807
9.898	3.39E-04	10.908	8.94063
9.951	3.57E-04	10.962	8.97185
10.003	8.67E-04	11.017	8.82533
10.056	0.00224	11.072	8.924
10.109	0.00667	11.127	9.49413
10.162	0.03198	11.183	9.57737
10.214	0.1421	11.236	9.83922
10.268	0.56388	11.288	9.82301
10.322	1.4617	11.337	10.23643
10.378	2.58255	11.391	10.0119
10.43	3.65094	11.44	10.4711
10.483	4.93549	11.494	10.75402

## Section 5: Model validation against IDT reported in this literature

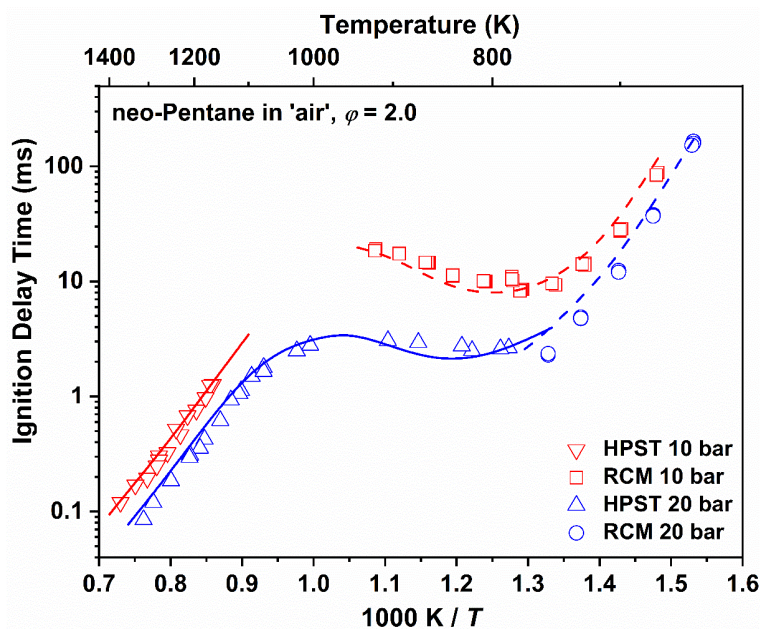
**Figure S11.** Measured (symbols) and model-predicted (lines) IDTs of neopentane at  $\phi = 0.5$ . The 10 atm (red) and 20 atm (blue) for neopentane in 'air'. Experimental data is taken from Bugler et al.<sup>3</sup> HPST: TAMU shock tube hardware, RCM: NUIG rapid compression machine.



**Figure S12.** Measured (symbols) and model-predicted (lines) IDTs of neopentane at  $\phi = 1$ . The 10 atm (red) and 20 atm (blue) for neopentane in 'air'. Experimental data is taken from Bugler et al.<sup>3</sup> HPST: TAMU shock tube hardware, RCM: NUIG rapid compression machine.



**Figure S13.** Measured (symbols) and model-predicted (lines) IDTs of neopentane at  $\phi = 2$ . The 10 atm (red) and 20 atm (blue) for neopentane in 'air'. Experimental data is taken from Bugler et al.<sup>3</sup> HPST: TAMU shock tube hardware, RCM: NUIG rapid compression machine.



## References

- (1) Dong, S.; Aul, C.; Gregoire, C.; Cooper, S. P.; Mathieu, O.; Petersen, E. L.; Rodriguez, J.; Mauss, F.; Wagnon, S. W.; Kukkadapu, G.; et al. A comprehensive experimental and kinetic modeling study of 1-hexene. *Combust. Flame* **2021**, 232.
- (2) Dagaut, P.; Cathonnet, M. Oxidation of neopentane in a jet-stirred reactor from 1 to 10 atm: an experimental and detailed kinetic modeling study. *Combust. Flame* **1999**, 118 (1), 191-203.
- (3) Bugler, J.; Marks, B.; Mathieu, O.; Archuleta, R.; Camou, A.; Grégoire, C.; Heufer, K. A.; Petersen, E. L.; Curran, H. J. An ignition delay time and chemical kinetic modeling study of the pentane isomers. *Combust. Flame* **2016**, 163, 138-156.