

Insights into nitromethane combustion from detailed kinetic modeling – Pyrolysis experiments in jet stirred and flow reactors

Krishna Prasad Shrestha¹, Nicolas Vin², Olivier Herbinet², Lars Seidel^{3*}, Frédérique Battin-Leclerc², Thomas Zeuch⁴ and Fabian Mauss¹

1. Thermodynamics and Thermal Process Engineering, Brandenburg University of Technology, Siemens-Halske-Ring 8, 03046 Cottbus, Germany

2. Laboratoire Réactions et Génie des Procédés, CNRS, Université de Lorraine, BP 20451, 1 rue Grandville, 54000 Nancy, France.

3. LOGE Deutschland GmbH, Burger Chaussee 25, 03044 Cottbus, Germany

4. Institut für Physikalische Chemie, Georg-August-Universität Göttingen, Tammannstraße 6, 37077 Göttingen, Germany

Supplement Material

1. Flow reactor - pyrolysis

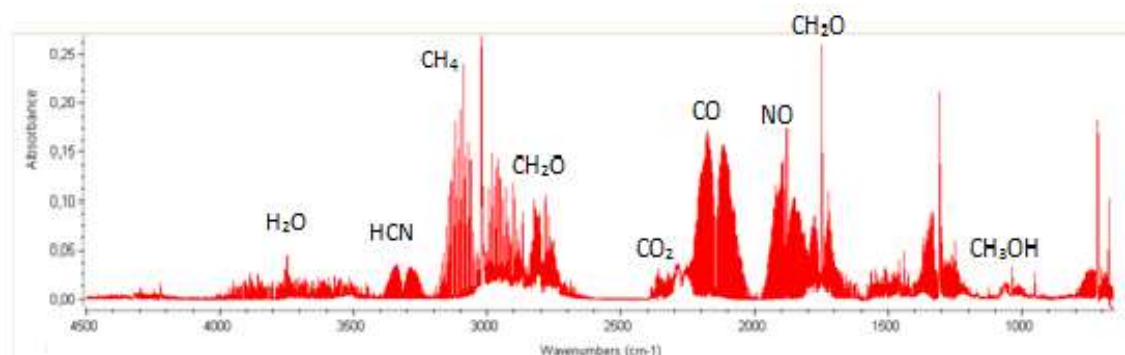


Figure S1: FTIR spectrum obtained during nitromethane pyrolysis.

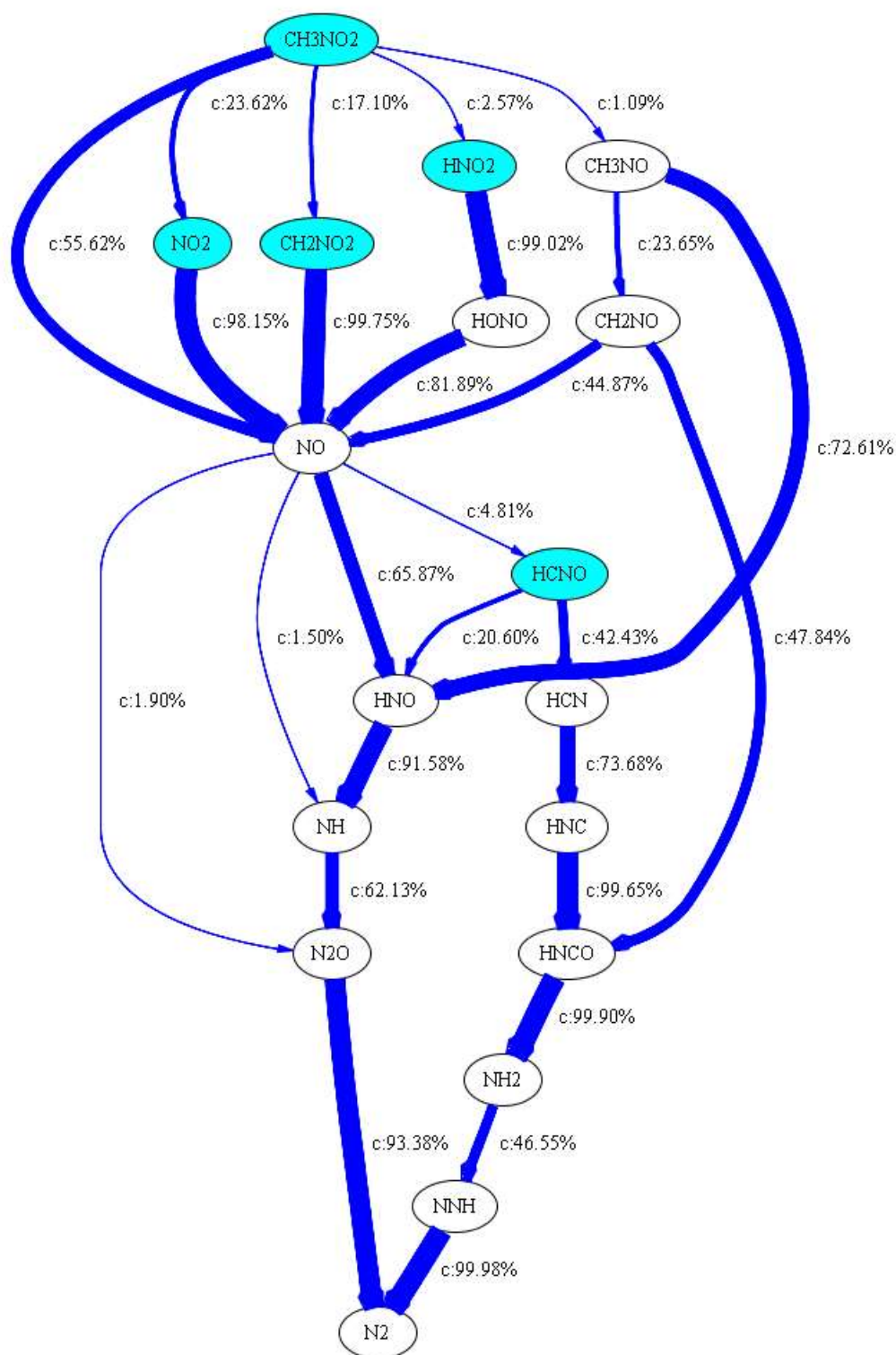


Figure S2: Integrated mass flux analysis for the pyrolysis of $\text{CH}_3\text{NO}_2/\text{Ar}$ in flow reactor shown in Figure 7. Based on the N-atom. CH_3NO_2 5 % / Ar 95 % (on a mole basis) at 5 Torr (= 0.666 kPa) , 1200 K at 30 % CH_3NO_2 consumption.

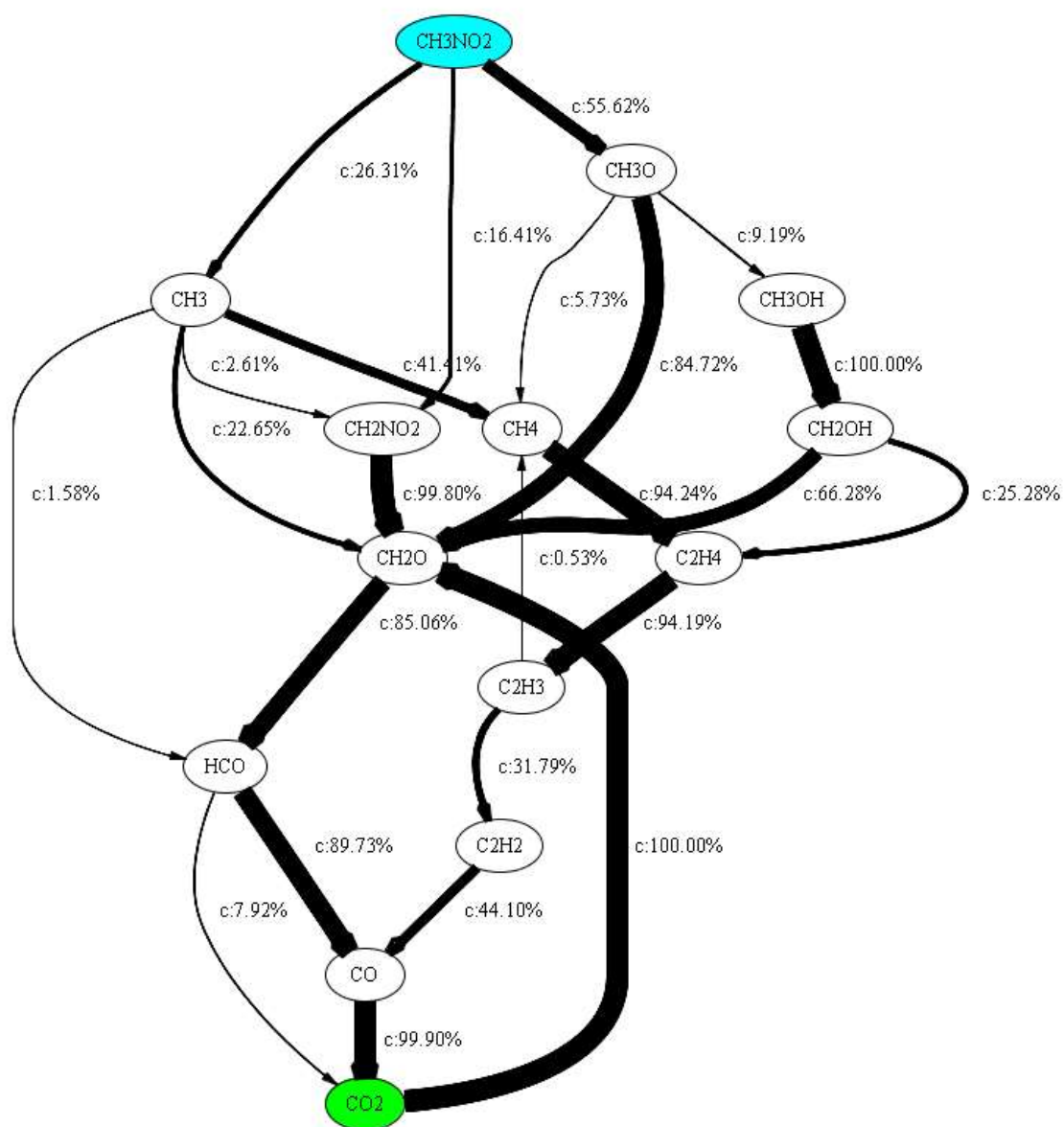


Figure S3: Integrated mass flux analysis for the pyrolysis $\text{CH}_3\text{NO}_2/\text{Ar}$ in flow reactor shown in Figure 7. Based on the C-atom. CH_3NO_2 5 % / Ar 95 % (on a mole basis) at 5 Torr (= 0.666 kPa), 1200 K at 30 % CH_3NO_2 consumption.

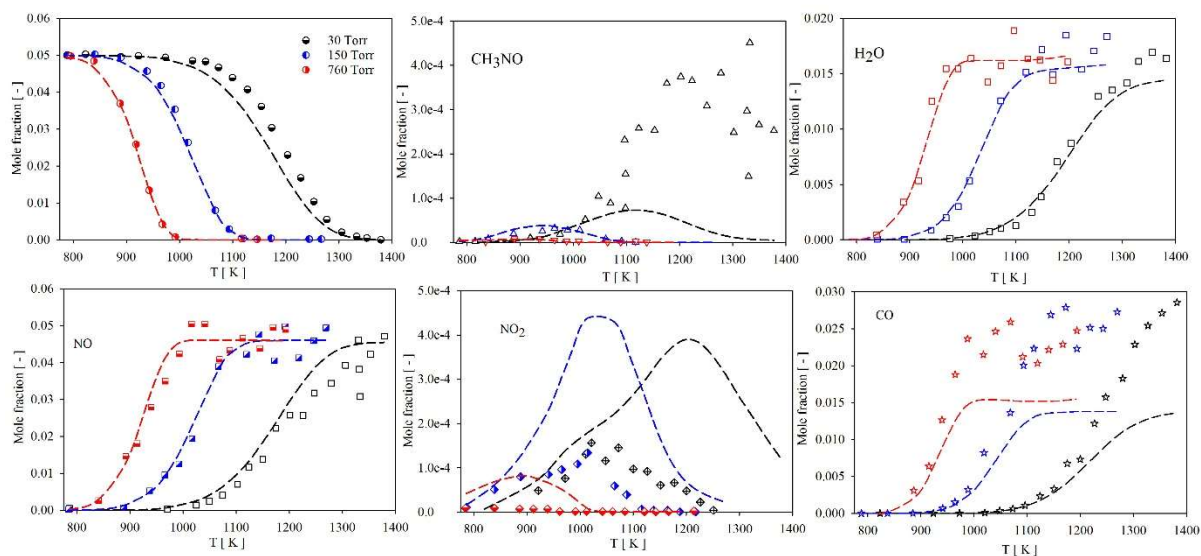


Figure S4: Pyrolysis of CH₃NO₂ 5 % / Ar 95 % in flow reactor at different pressures and residence times. Symbols: experimental data from [1], dashed lines: this model. Simulation are done using the temperature profile.

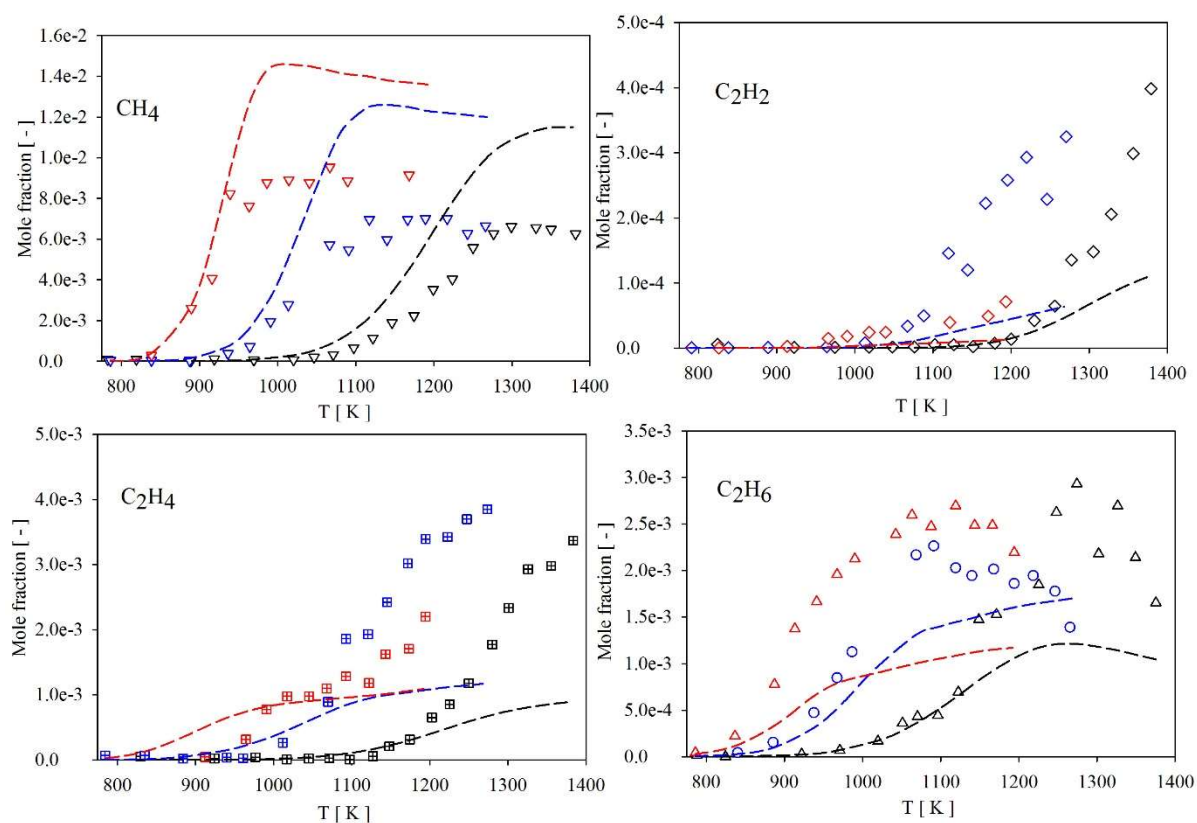


Figure S5: Pyrolysis of CH_3NO_2 5 % / Ar 95 % in flow reactor at different pressures and residence times. Symbols: experimental data from [1], dashed lines: this model. Simulation are performed imposing the temperature profile. Legend information same as in Figure S4.

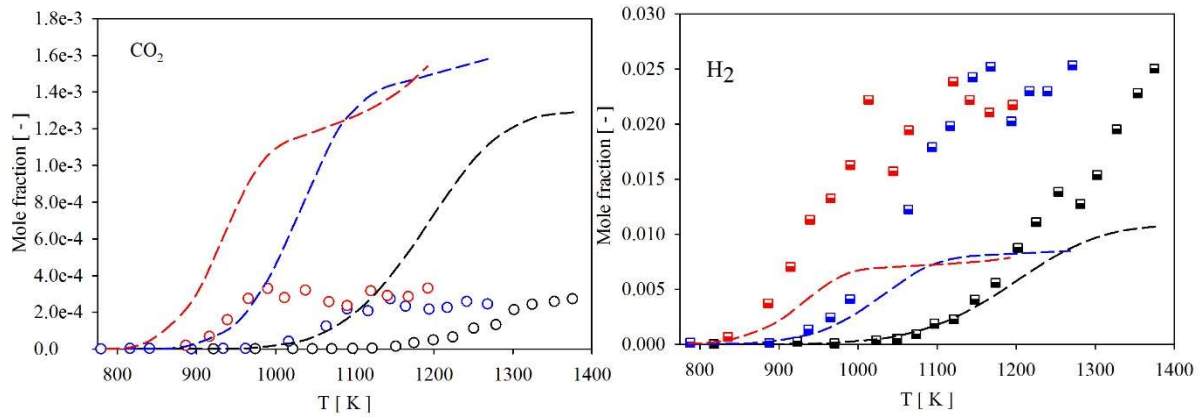


Figure S6: Pyrolysis of CH_3NO_2 5 % / Ar 95 % in flow reactor at different pressures and residence times. Symbols: experimental data from [1], dashed lines: this model. Simulation are performed imposing the temperature profile. Legend information same as in Figure S4.

2. Jet stirred reactor

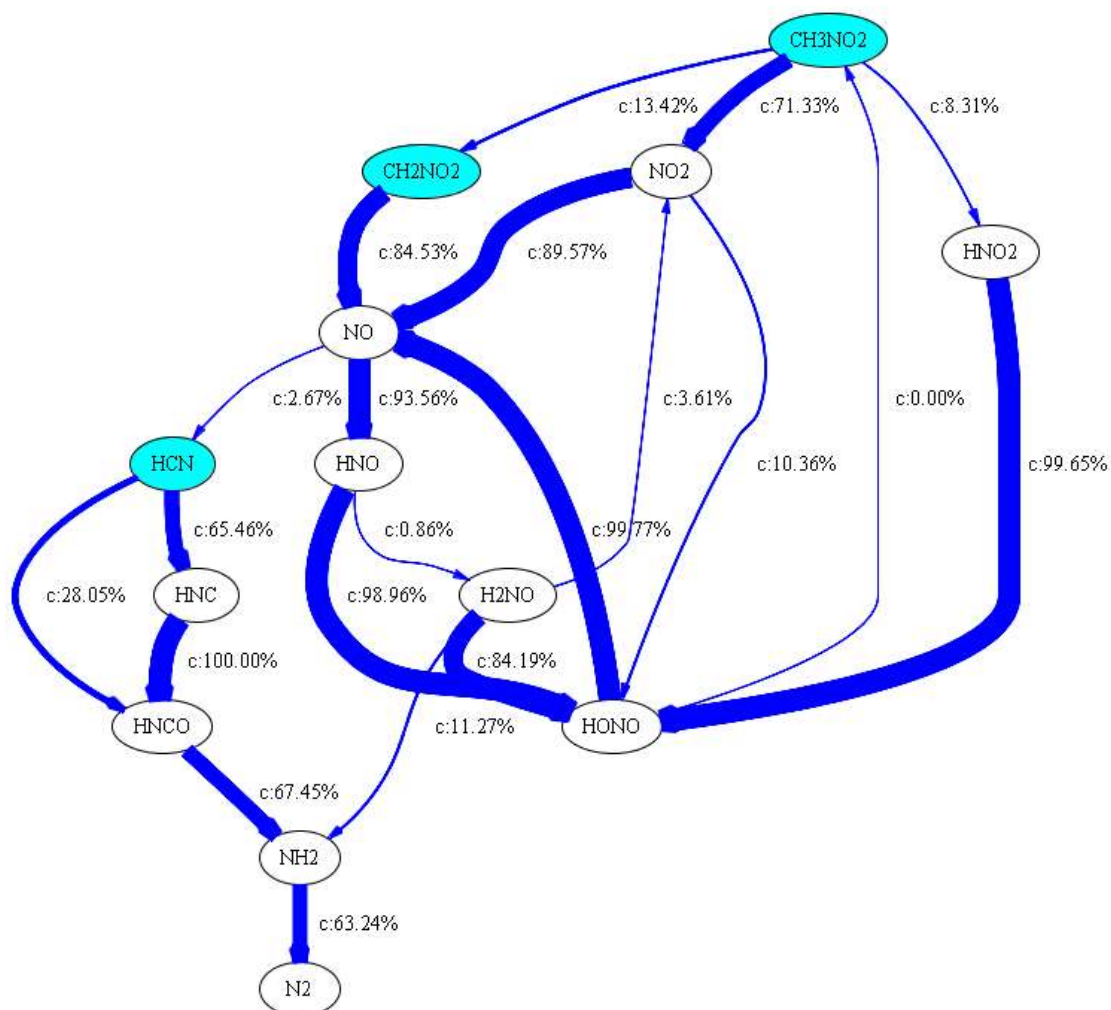


Figure S7: Integrated mass flux analysis during the pyrolysis of CH_3NO_2 1% / He 99% in JSR at 1.07 bar, $\tau = 2.0$ s for the condition shown in Figure 8. Based on N-atom.

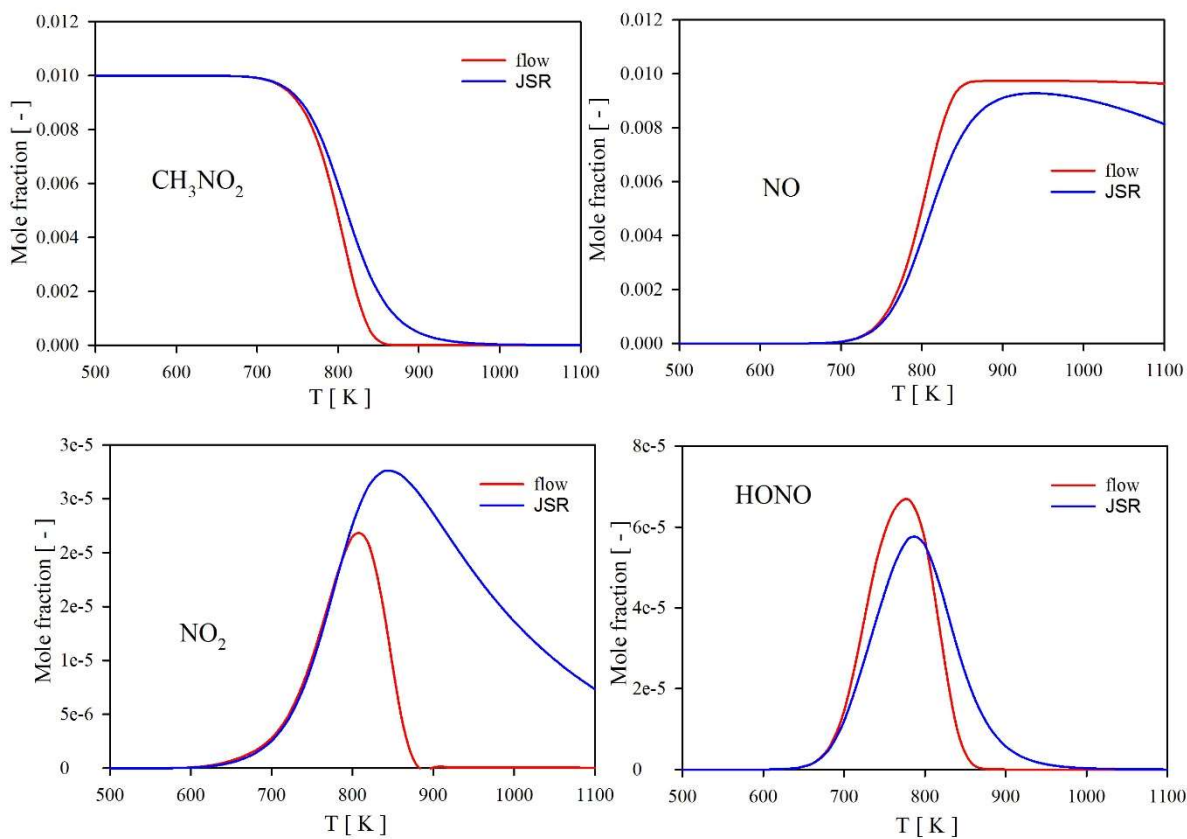


Figure S8: Species profile comparison during pyrolysis of CH₃NO₂ 1 % / He 99 % in flow reactor and JSR for the condition shown in Figure 3 and Figure 8 respectively. Red line: flow reactor, Blue line: JSR.

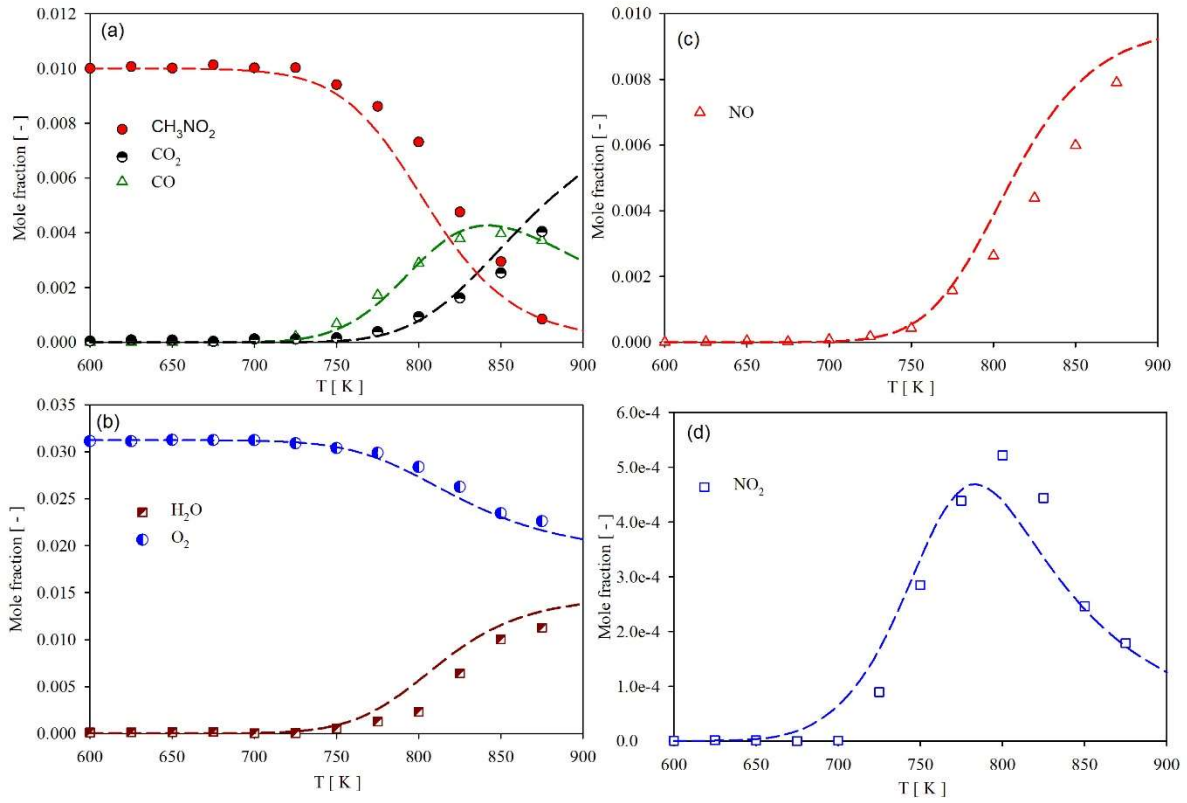


Figure S9: Oxidation of CH_3NO_2 1 % / O_2 3.125 % / Ar at 1 atm, $\phi = 0.4$, $\tau = 2.0$ s in a jet stirred reactor. Symbols: experimental data from Weng et al. [2]; dashed lines: this model.

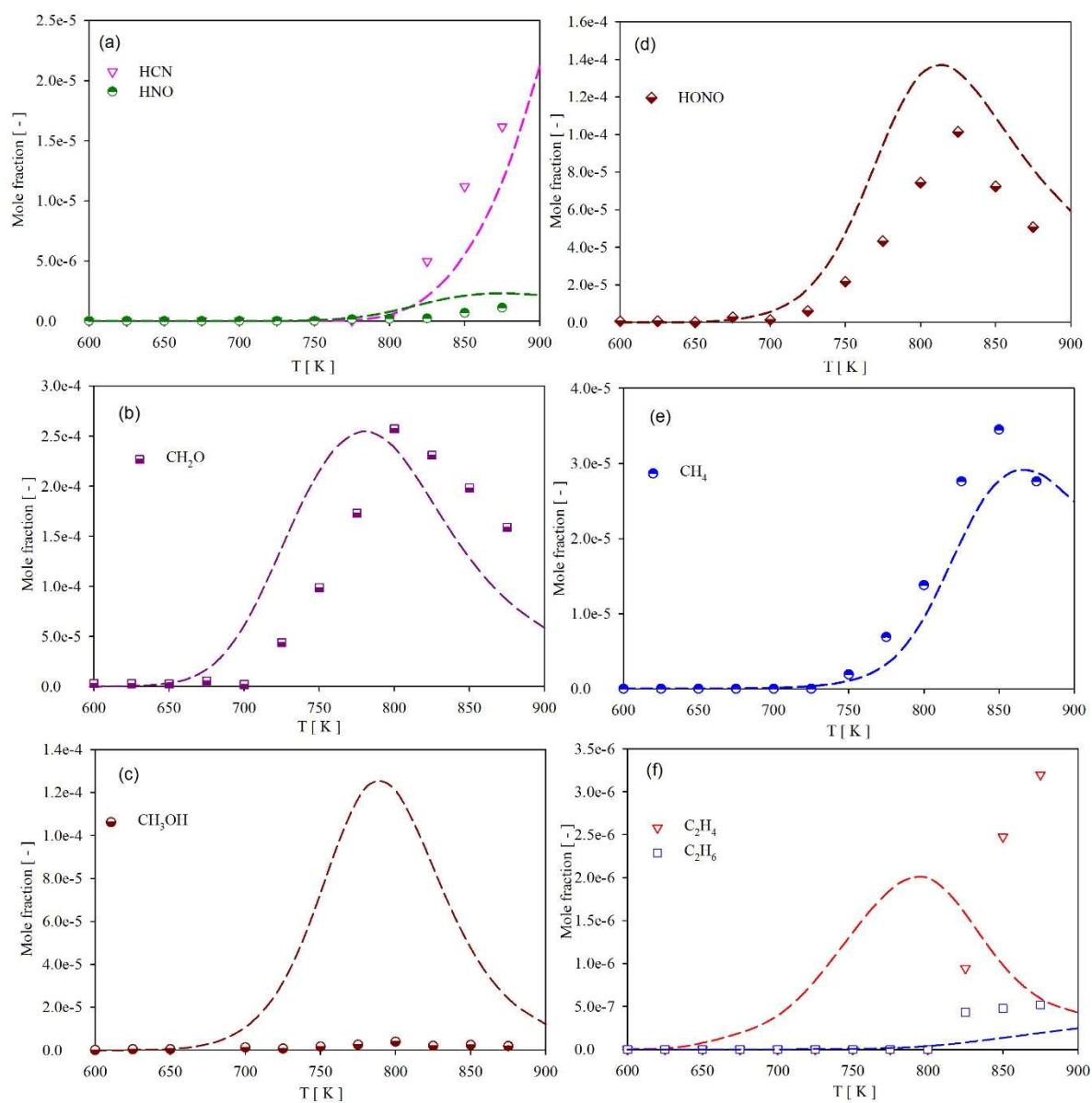


Figure S10: Oxidation of CH_3NO_2 1 % / O_2 3.125 % / Ar at 1 atm, $\phi = 0.4$, $\tau = 2.0$ s in a jet stirred reactor for condition in Figure S9. Symbols: experimental data from Weng et al. [2]; dashed lines: this model.

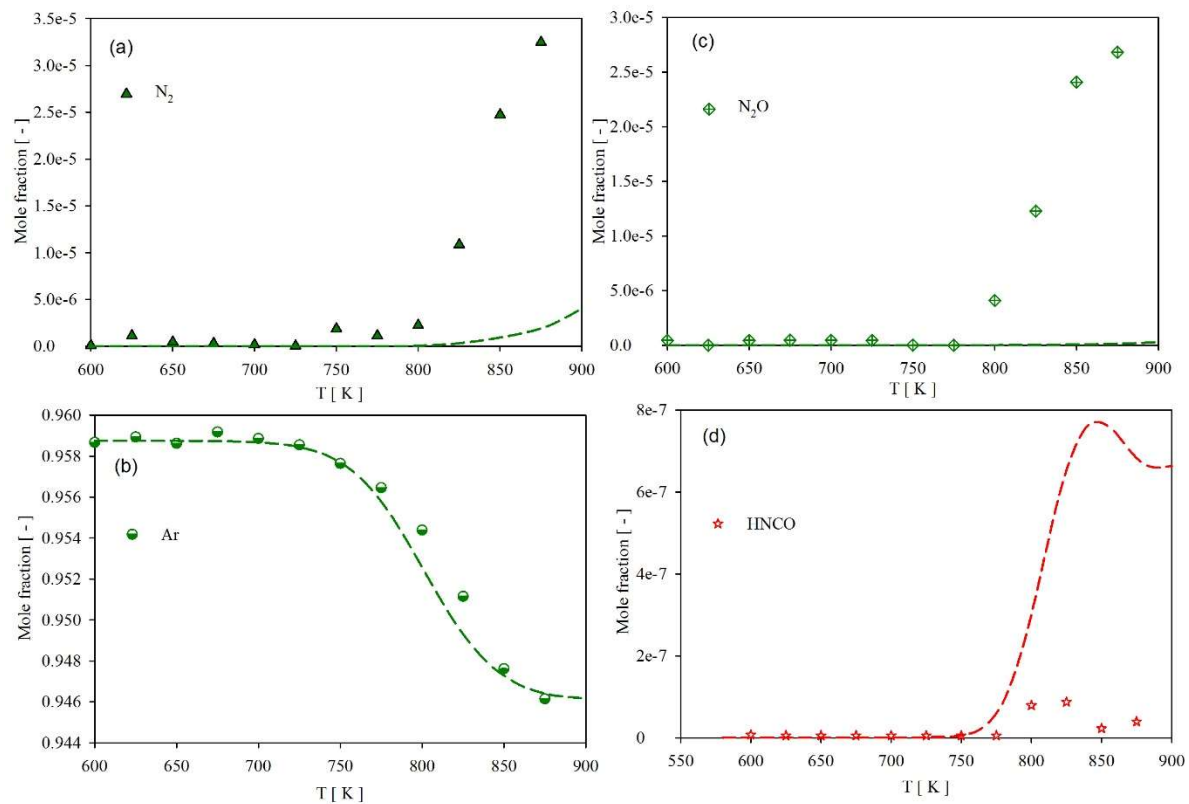


Figure S11: Oxidation of CH₃NO₂ 1 % / O₂ 3.125 % /Ar at 1 atm, $\phi = 0.4$, $\tau = 2.0$ s in a jet stirred reactor for condition in Figure S9. Symbols: experimental data from Weng et al. [2]; dashed lines: this model.

3. Burner stabilized flame

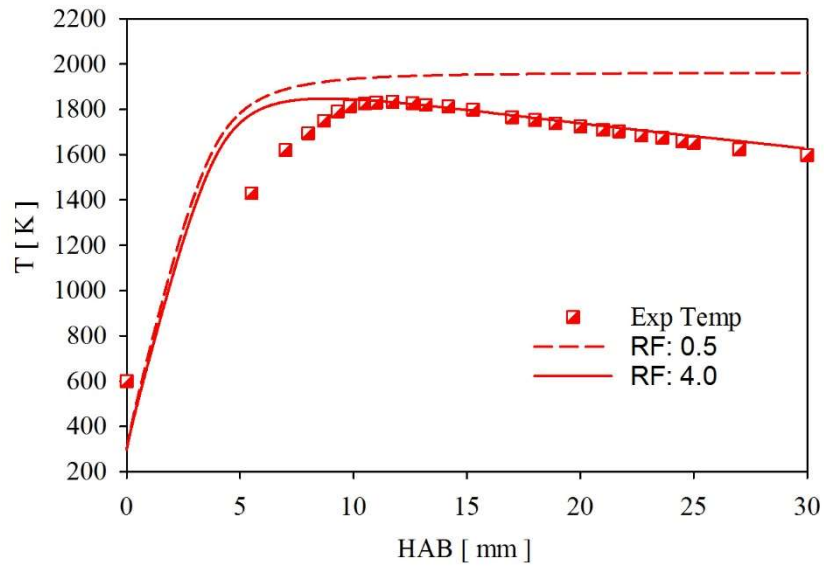


Figure S12: Temperature profile for the $\text{CH}_3\text{NO}_2/\text{O}_2/\text{Ar}$ premixed burner stabilized flame at 4.666 kPa, $T = 298$ K, $\phi = 1.5$ shown in Figure 15. Symbols: experiment measurement from [3], lines: calculation solving the energy conservation equation. Dash lines: with radiation factor (RF) 0.5 (standard setting), solid lines: with radiation factor (RF) 4.0.

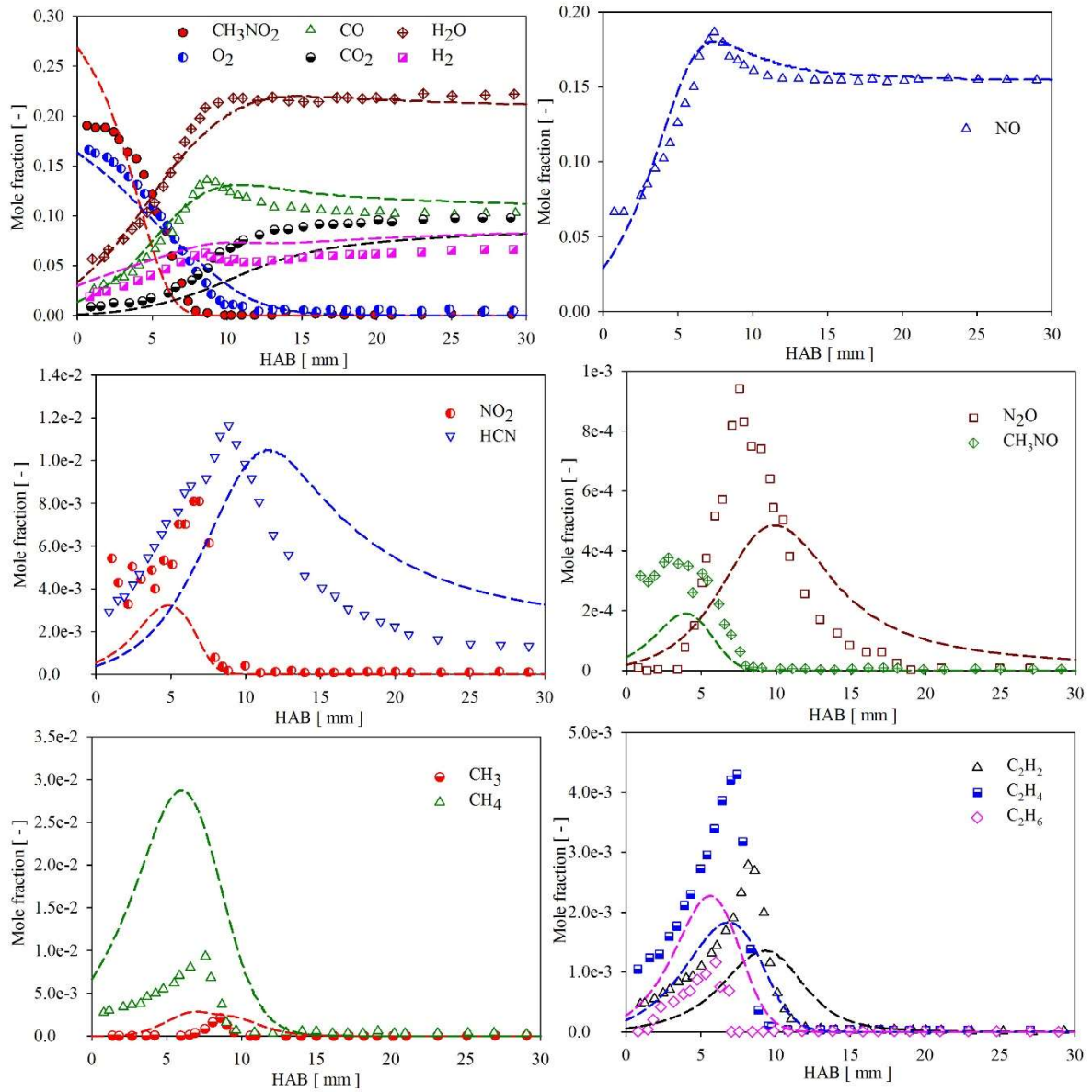


Figure S13: Speciation of premixed $\text{CH}_3\text{NO}_2/\text{O}_2/\text{Ar}$ burner stabilized flame at 4.666 kPa, $T = 298 \text{ K}$, $\phi = 2.0$. Symbols: experiments from Zhang et al. [3]; dashed lines: prediction imposing the experimental temperature profile.

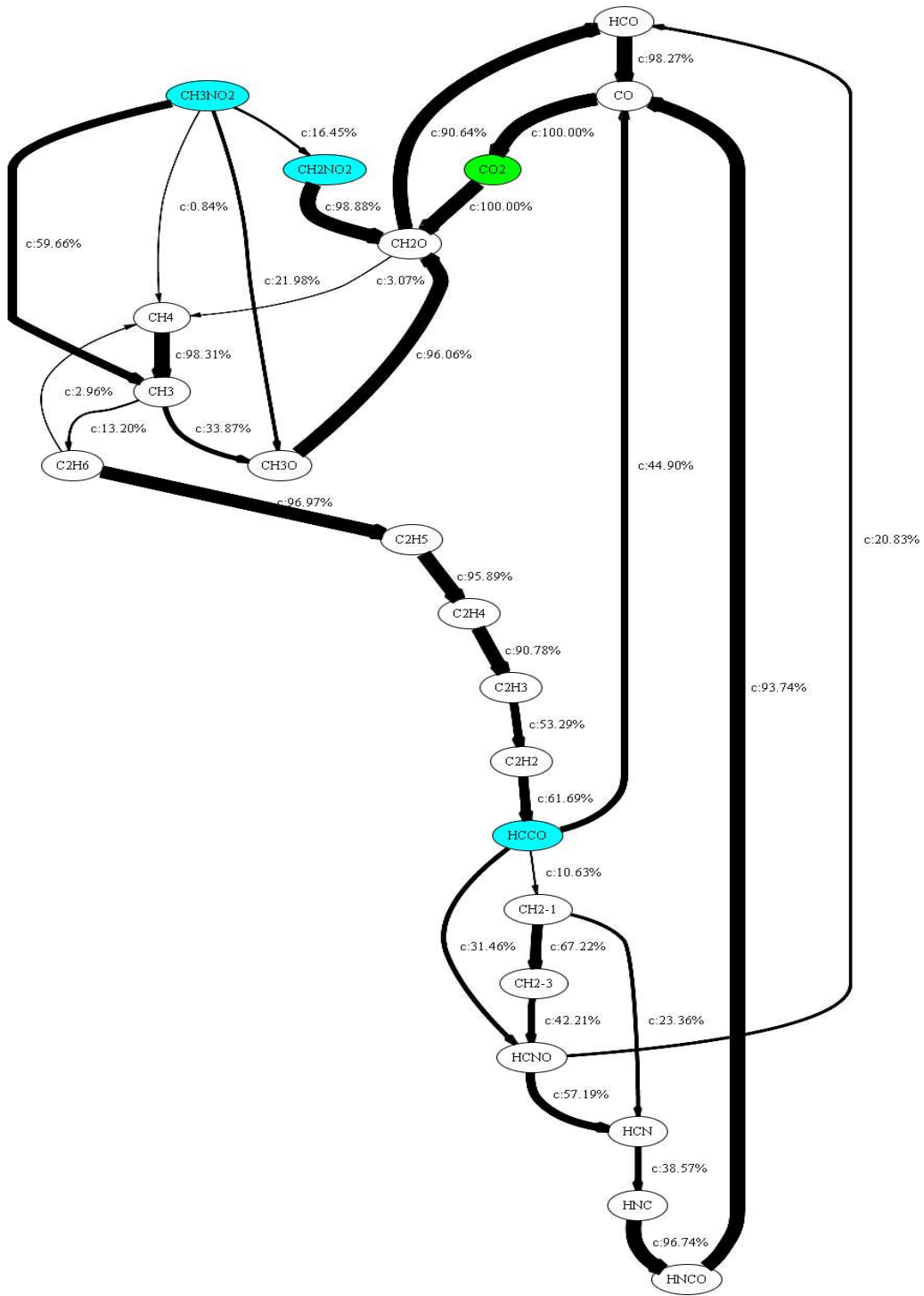


Figure S14: Integrated mass flux analysis for CH₃NO₂/O₂/Ar burner stabilized flame at 4.666 kPa, T = 298 K, $\phi = 2.0$ shown in Figure S13. Based on the C-atom.

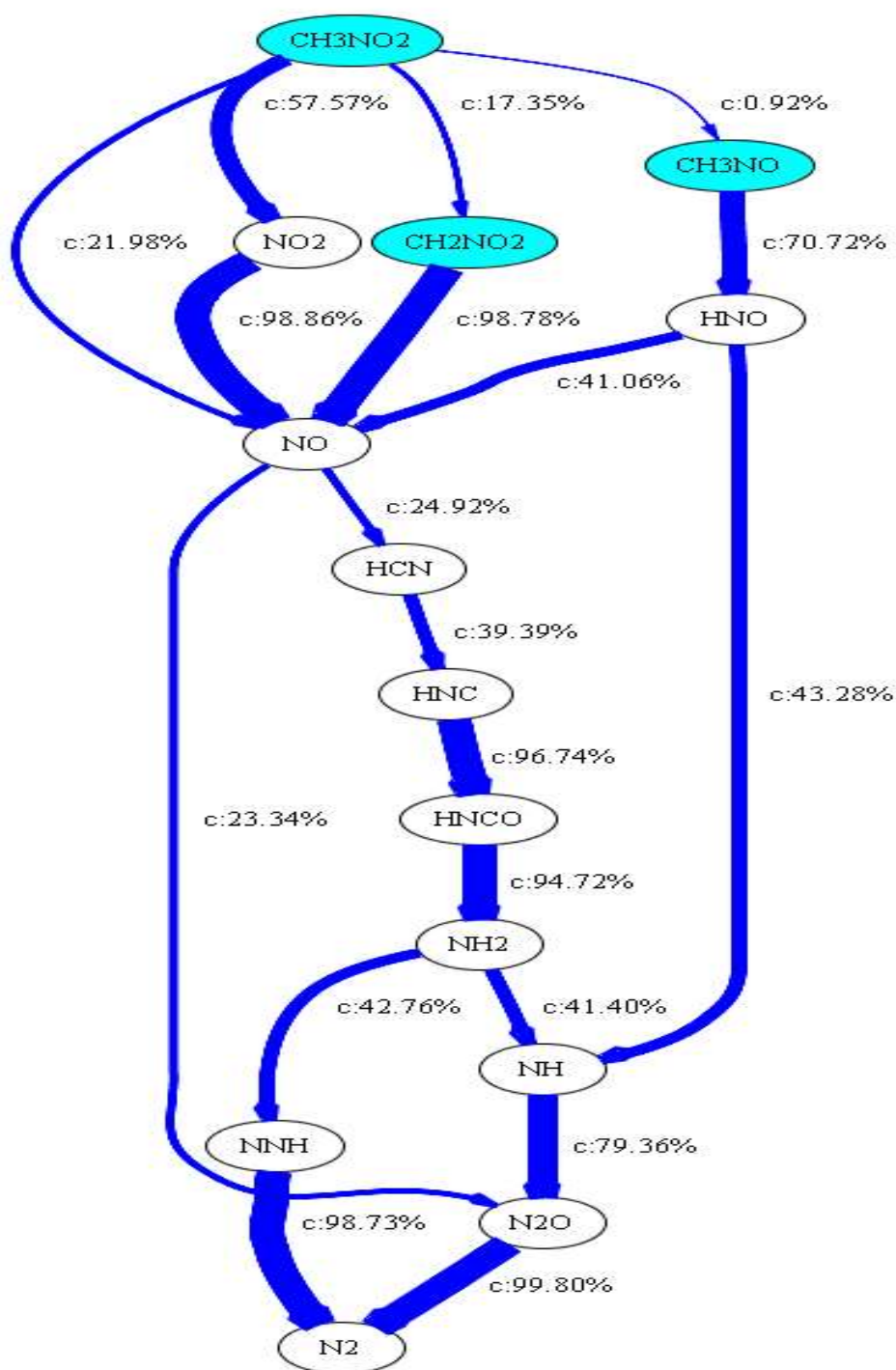


Figure S15: Integrated mass flux analysis for CH₃NO₂/O₂/Ar burner stabilized flame at 4.666 kPa, T = 298 K, $\phi = 2.0$ shown in Figure S13. Based on the N-atom.

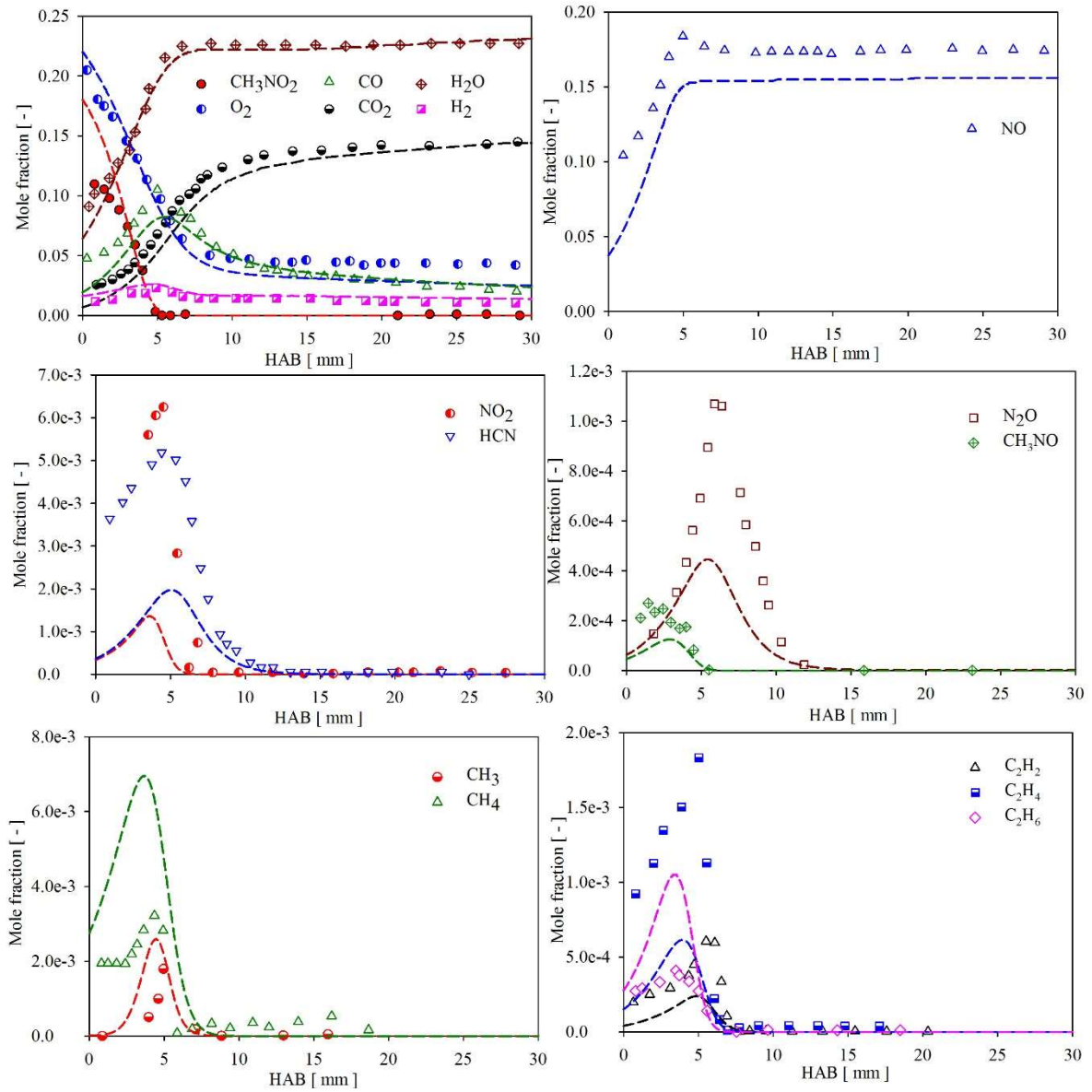


Figure S16: Speciation of premixed $\text{CH}_3\text{NO}_2/\text{O}_2/\text{Ar}$ burner stabilized flame at 4.666 kPa, $T = 298 \text{ K}$, $\phi = 1.0$. Symbols: experiments from Zhang et al. [3]; dashed lines: prediction imposing the experimental temperature profile.

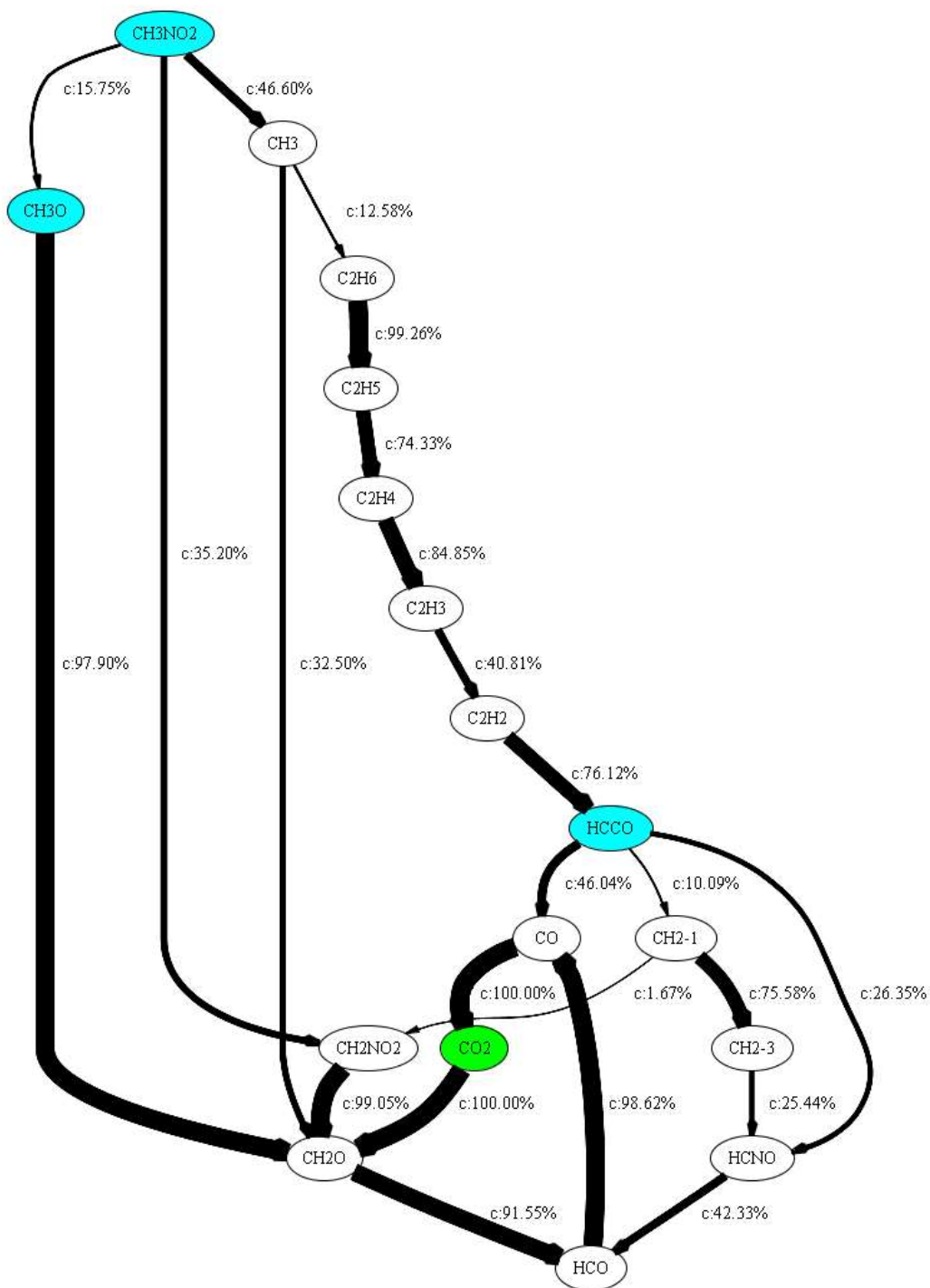


Figure S17: Integrated mass flux analysis for $\text{CH}_3\text{NO}_2/\text{O}_2/\text{Ar}$ burner stabilized flame at 4.666 kPa, $T = 298$ K, $\phi = 1.0$ shown in Figure S16. Based on the C-atom.

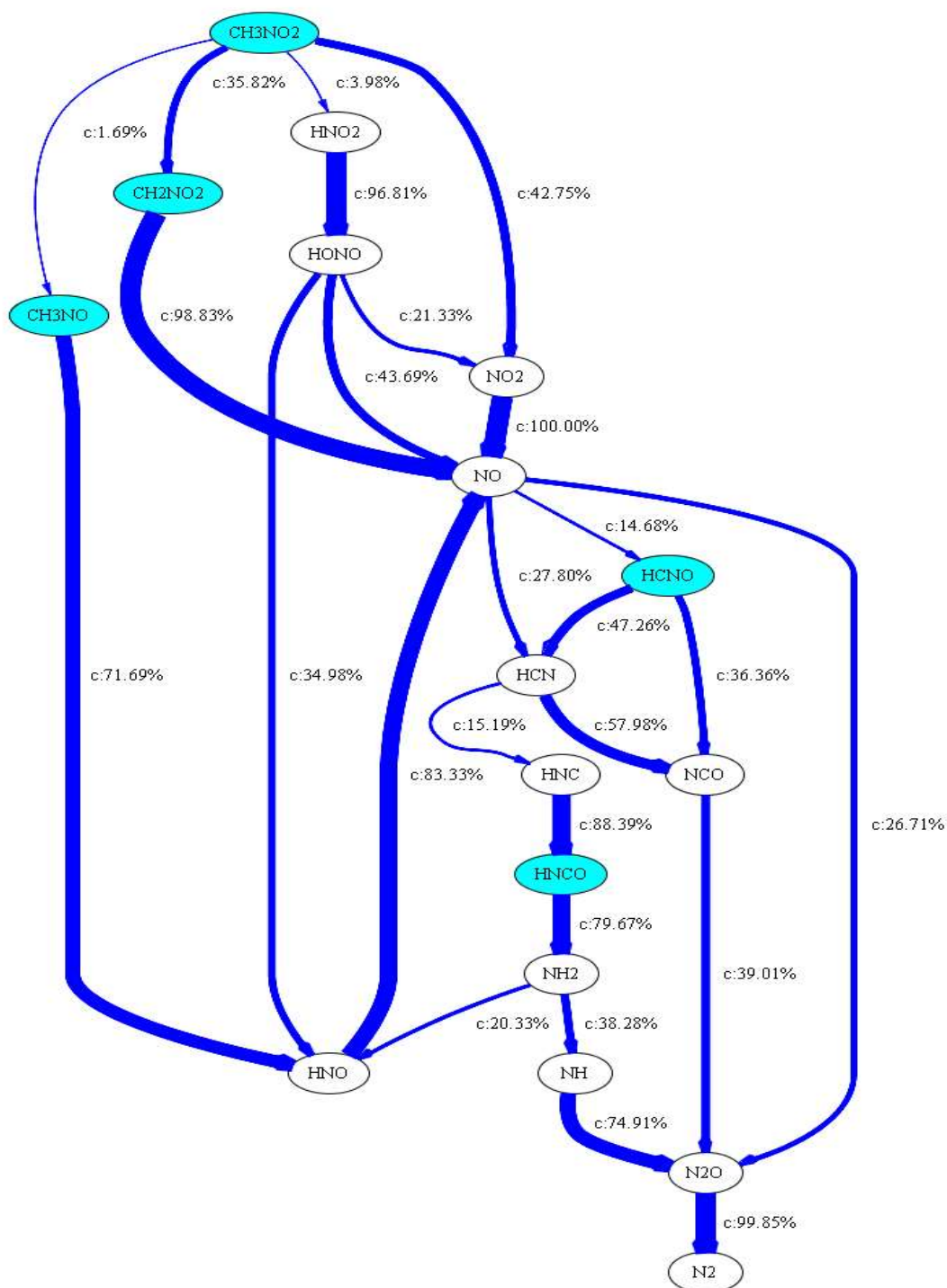


Figure S18: Integrated mass flux analysis for CH₃NO₂/O₂/Ar burner stabilized flame at 4.666 kPa, T = 298 K, $\phi = 1.0$ shown in Figure S16. Based on the N-atom.

4. Shock tube - Ignition delay time and pyrolysis

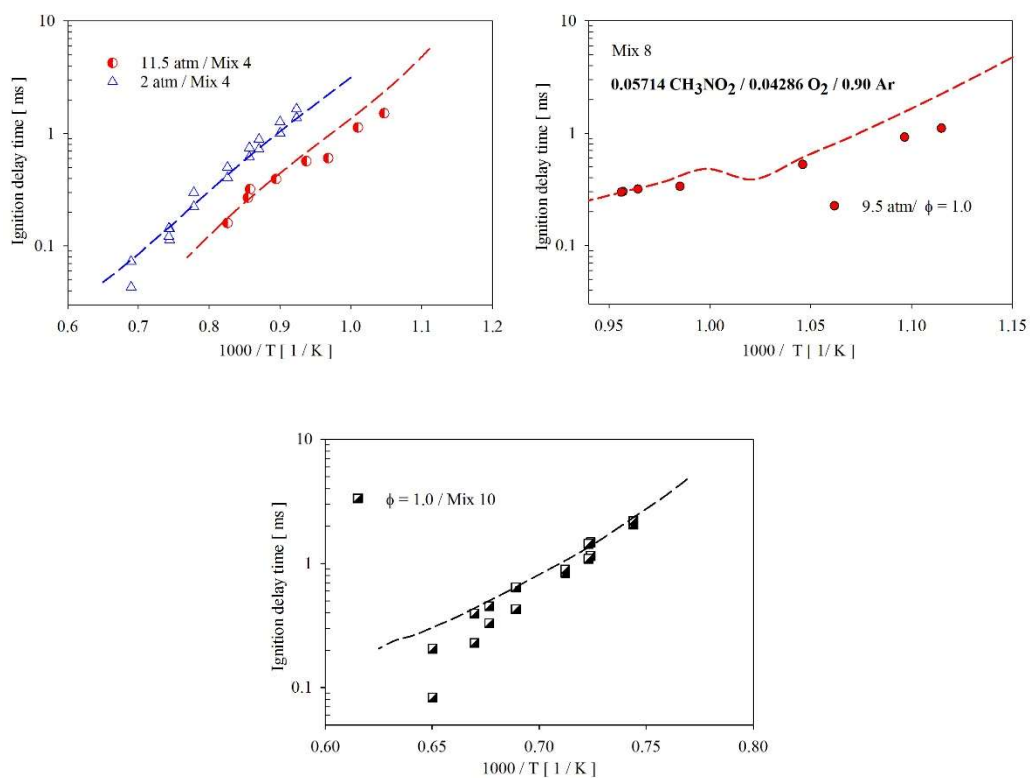


Figure S19: Ignition delay time of $\text{CH}_3\text{NO}_2/\text{O}_2/\text{Ar}$. Symbols: experiment from Mathieu et al. 2016 [4]; lines: this model. Mix: means mixture number, which is same as in [4].

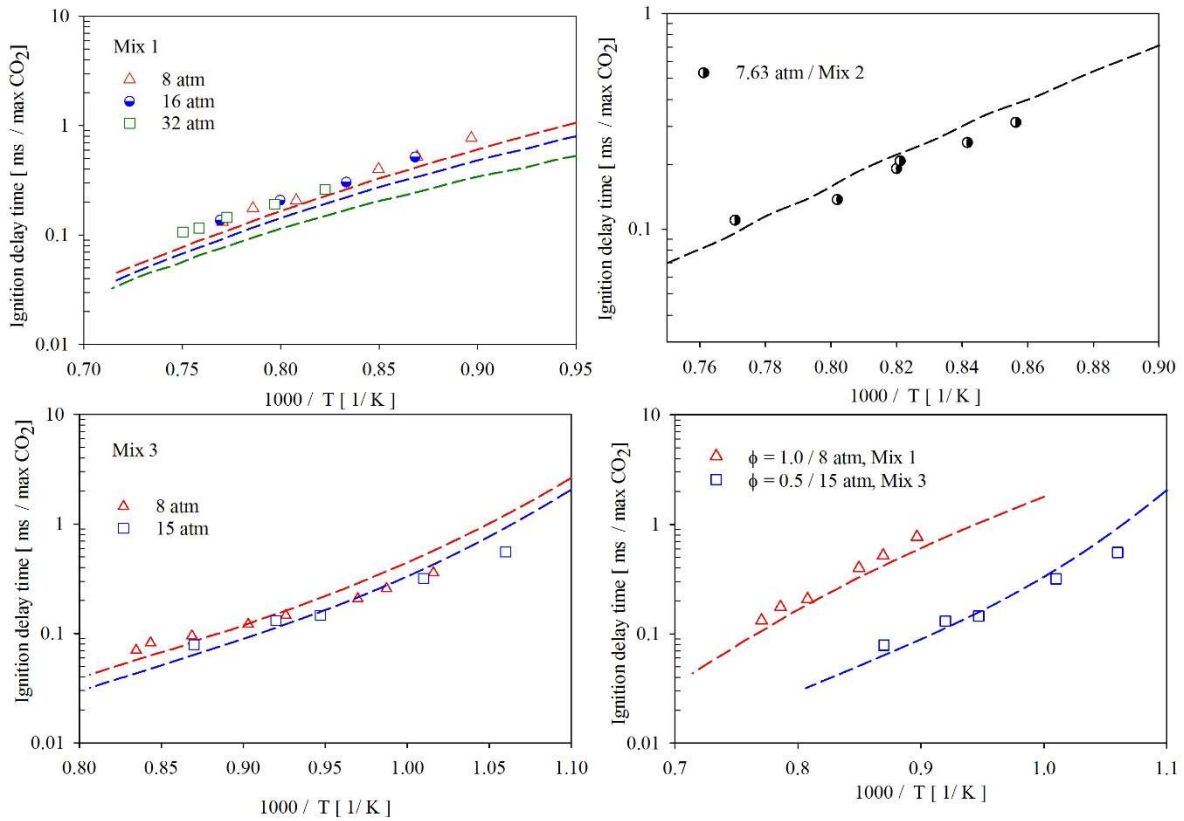


Figure S20: Ignition delay times of CH₃NO₂/O₂/N₂. Symbols: experiment from Nauc \acute{e} l et al. 2016 [5]; lines: this model. Mix: means mixture number, which is same as in [5].

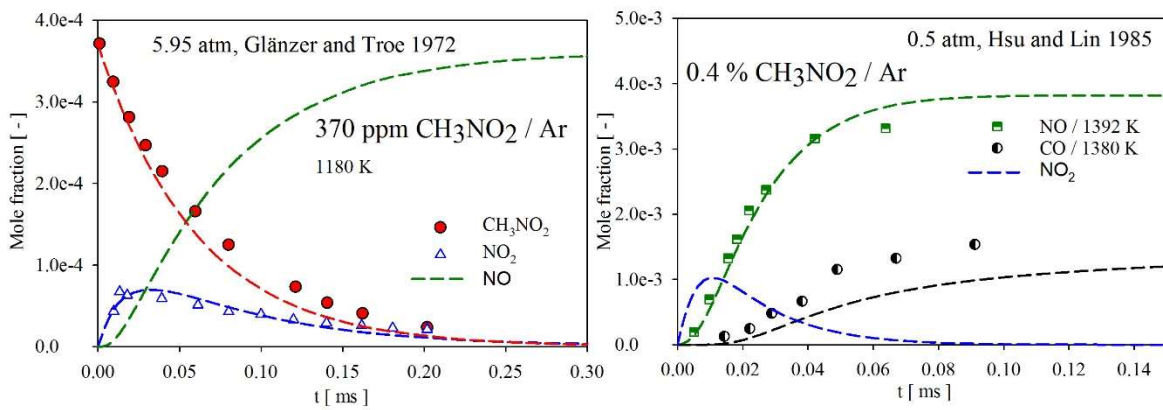


Figure S21: Speciation during the CH₃NO₂/Ar pyrolysis in shock tube, symbols: experiments from [6] (left), [7] (right); lines: this model.

5. Laminar flame speed

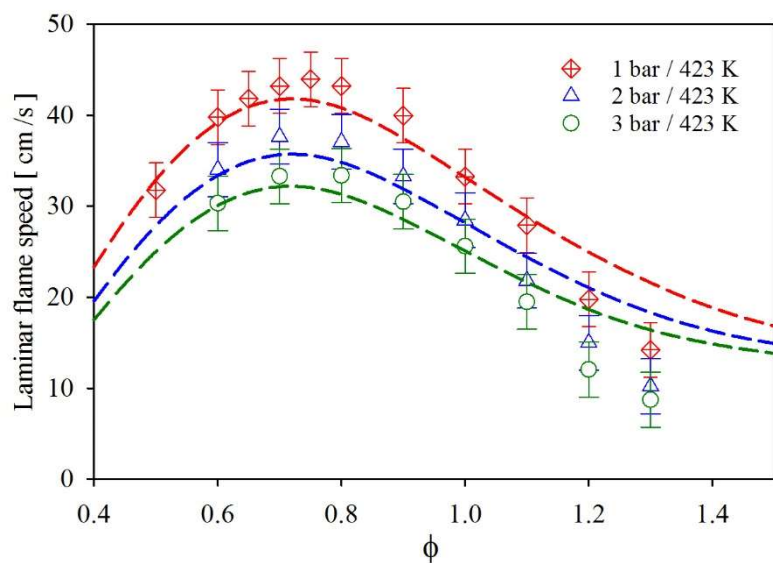


Figure S22: Laminar flame speeds of $\text{CH}_3\text{NO}_2/\text{air}$ at 423 K and three different pressures (1–3 bar). Symbols: experiment from [8]; lines: this model.

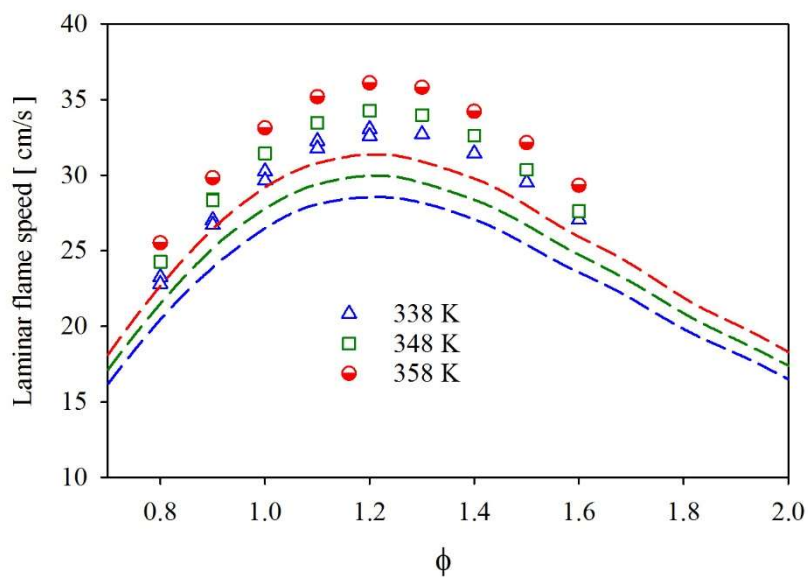


Figure S23: Laminar flame speed of $\text{CH}_3\text{NO}_2/\text{air}$ at 1 atm and three different temperatures. Symbols: experiment from [9]; lines: this model.

6. $\text{CH}_3\text{NO}_2(+\text{M}) \rightleftharpoons \text{CH}_3 + \text{NO}_2(+\text{M})$ rate constant comparison

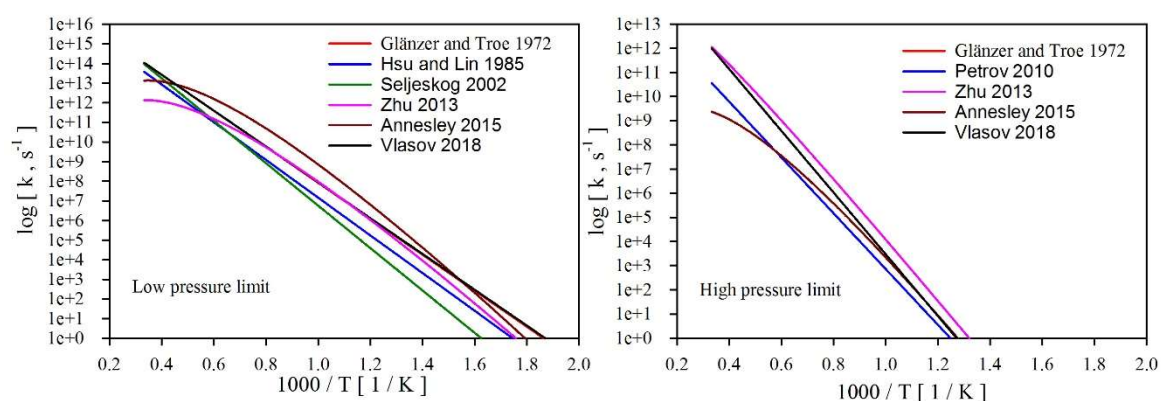


Figure S24: Rate constant comparison of reaction $\text{CH}_3\text{NO}_2(+\text{M}) \rightleftharpoons \text{CH}_3 + \text{NO}_2(+\text{M})$ from different sources: Glänzer and Troe [6], Hsu and Lin [7], Seljeskog [10], Zhu et al. [11], Annesley et al. [12], Vlasov et al. [13], Petrov et al. [14].

References

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