On the implications of nitromethane - NO_x chemistry interactions for combustion processes

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Supplementary Material

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The detailed reaction mechanism provided as the supplement to this work includes both hydrocarbon and nitrogen chemistry. The mechanism also considers ammonia (NH_3) as a fuel. In addition to fuel/NO_x system mechanism can also be used to simulate the fuel blend with NH_3.

1. CH_4 oxidation doped with NO and NO_2

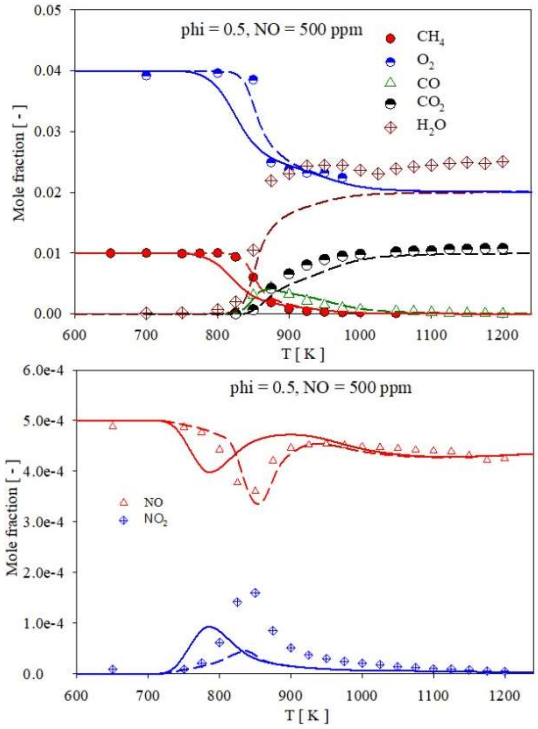

Figure S1: Oxidation of $CH_4/O_2/Ar$ doped with 500 ppm of NO in a JSR at ϕ = 0.5 and 1.07 bar. Symbols: experimental data from [1], Dashed lines: with CH_3NO_2 chemistry, Solid lines: without CH_3NO_2 chemistry.

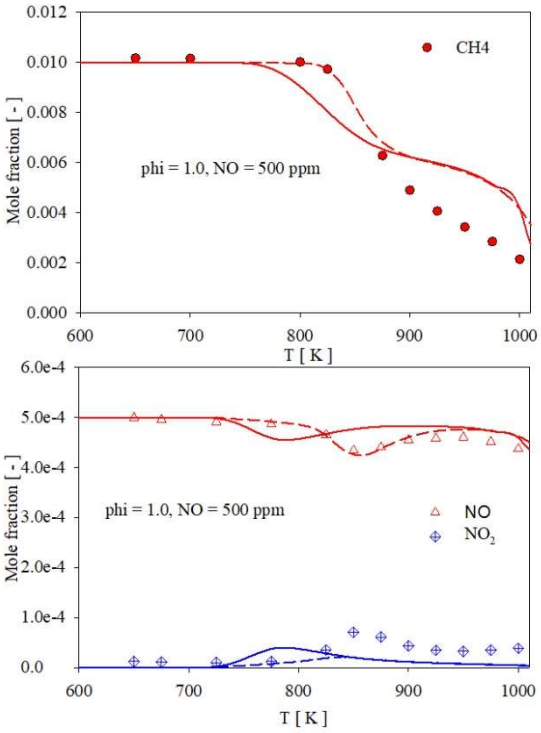

Figure S2: Oxidation of $CH_4/O_2/Ar$ doped with 500 ppm of NO in a JSR at ϕ = 1.0 and 1.07 bar. Symbols: experimental data from [1], Dashed lines: with CH_3NO_2 chemistry, Solid lines: without CH_3NO_2 chemistry.

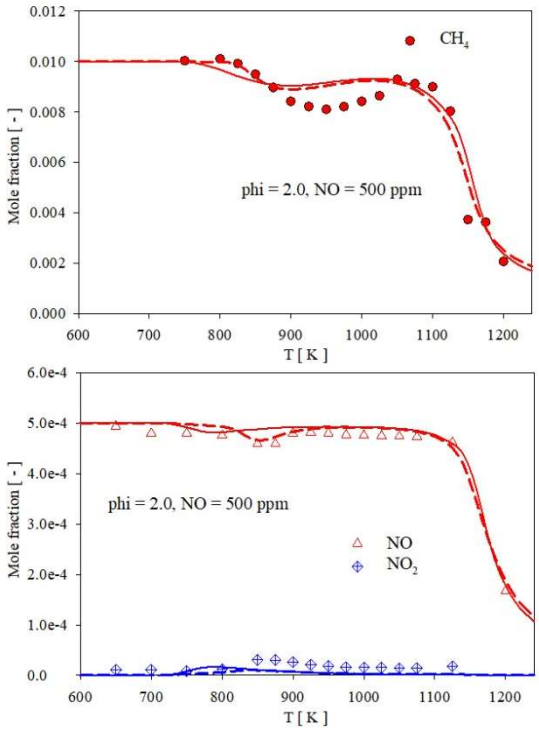

Figure S3: Oxidation of $CH_4/O_2/Ar$ doped with 500 ppm of NO in a JSR at $\phi = 2.0$ and 1.07 bar. Symbols: experimental data from [1], Dashed lines: with CH_3NO_2 chemistry, Solid lines: without CH_3NO_2 chemistry.

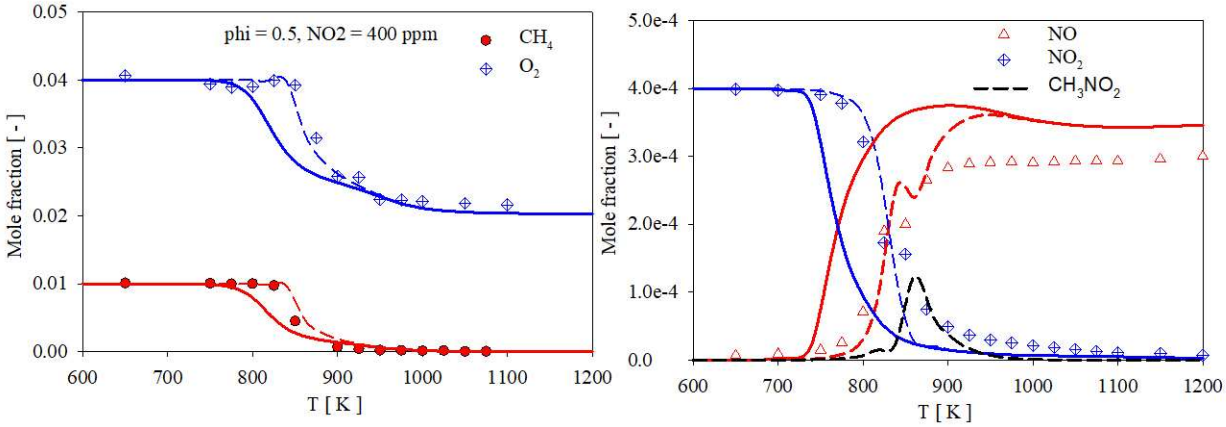

Figure S4: Oxidation of $CH_4/O_2/Ar$ doped with 400 ppm of NO_2 in a JSR at $\phi = 0.5$ and 1.07 bar. Symbols: experimental data from [1], Dashed lines: with CH_3NO_2 chemistry, Solid lines: without CH_3NO_2 chemistry.

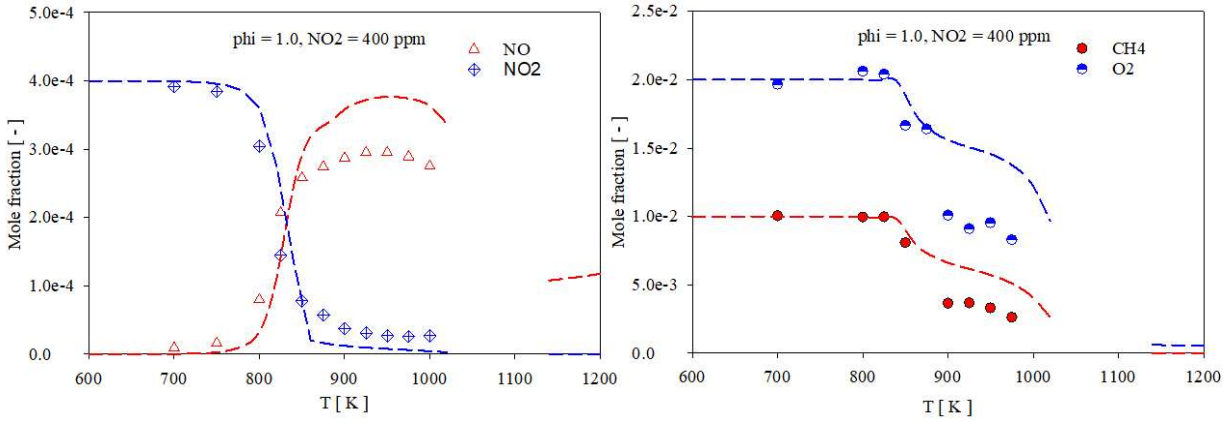

Figure S5: Oxidation of $CH_4/O_2/Ar$ doped with 400 ppm of NO_2 in a JSR at ϕ = 1.0 and 1.07 bar. Symbols: experimental data from [1], Dashed lines: with CH_3NO_2 chemistry, Solid lines: without CH_3NO_2 chemistry.

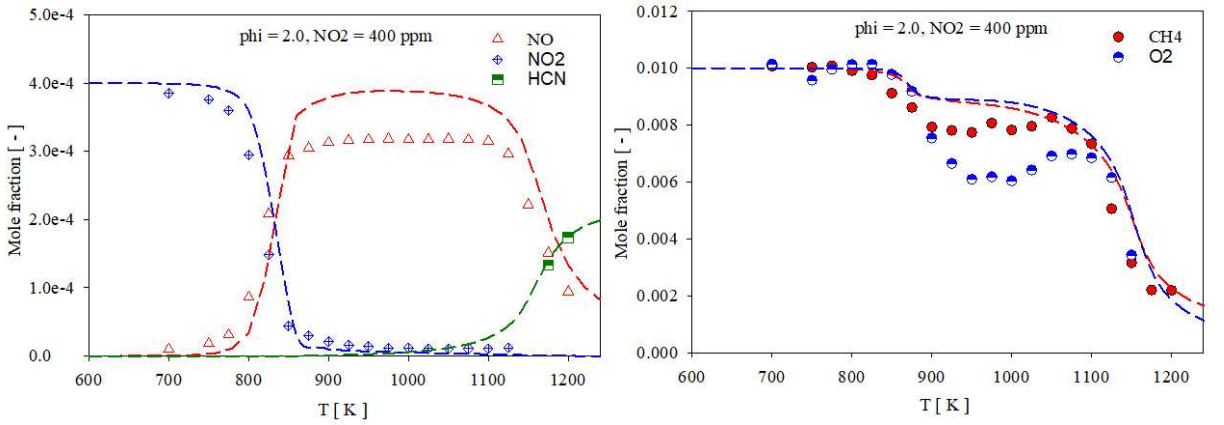

Figure S6: Oxidation of $CH_4/O_2/Ar$ doped with 400 ppm of NO_2 in a JSR at ϕ = 2.0 and 1.07 bar. Symbols: experimental data from [1], Dashed lines: with CH_3NO_2 chemistry, Solid lines: without CH_3NO_2 chemistry.

2. n-Heptane oxidation doped with and without NO

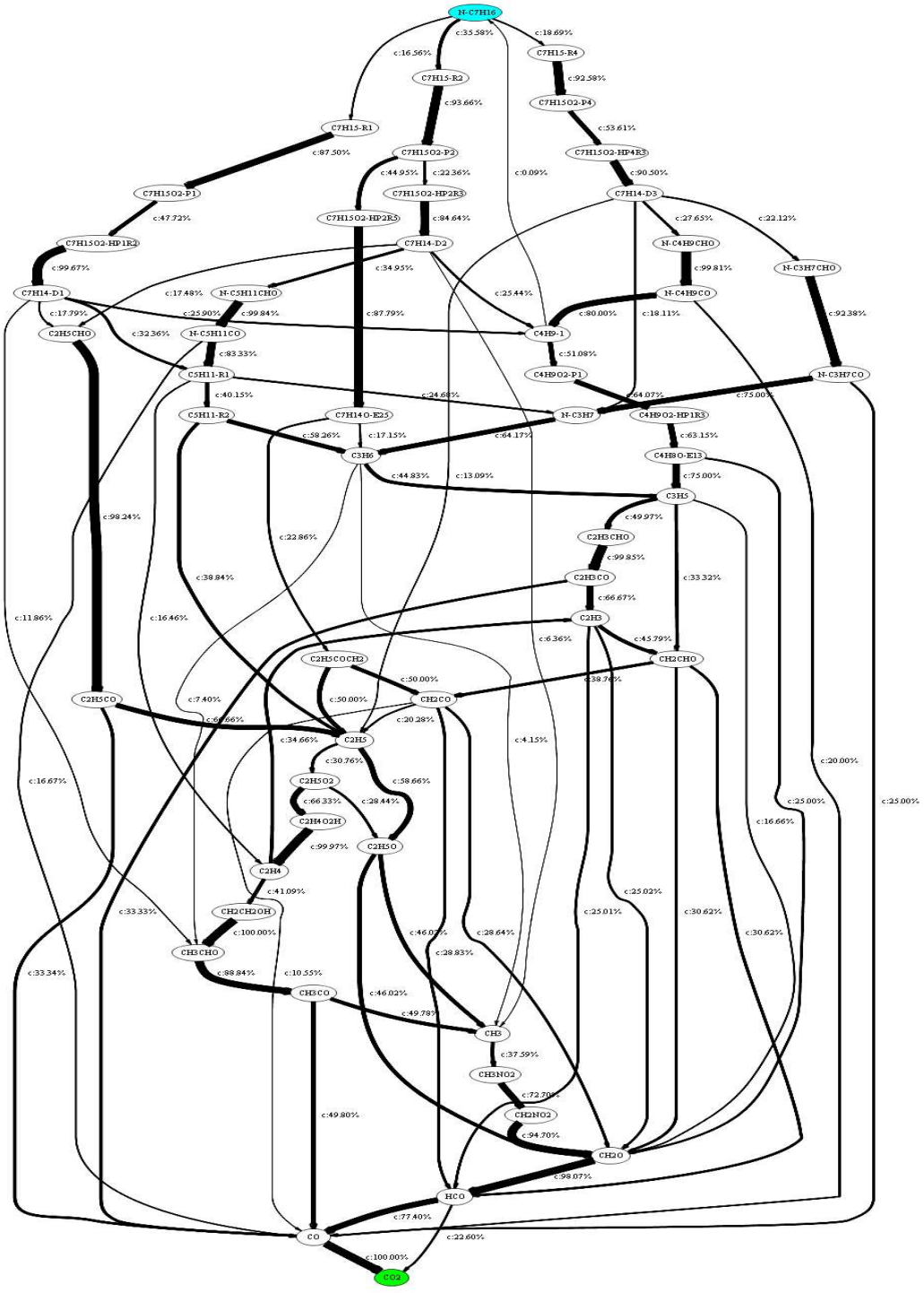

Figure S7: Reaction path analysis for n-C7H16/O2/N2/NO (500 ppm) based on C-atom at 740 K, 10 atm, ϕ = 1.0 and τ = 1.0 s.

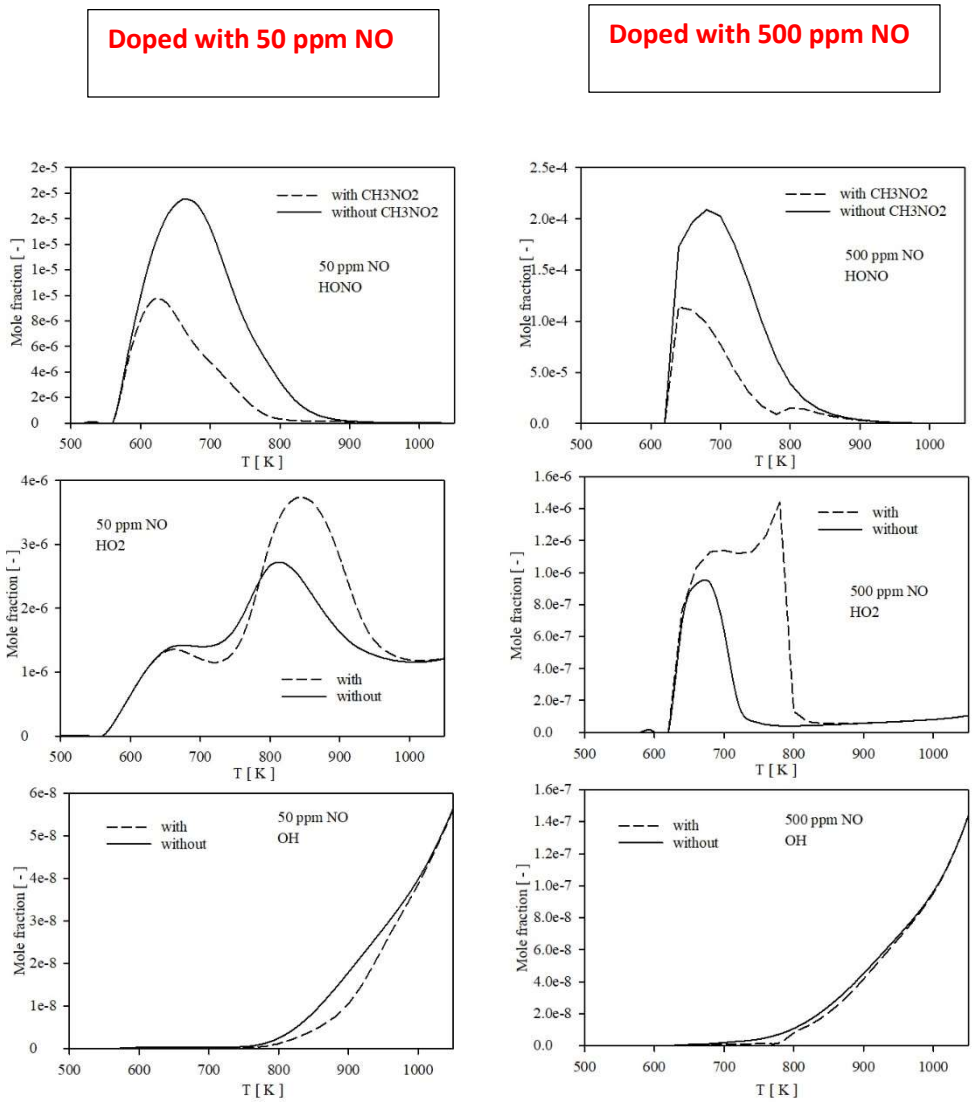

Figure S8: HONO, HO_2 and OH concentration profiles during Oxidation of n-$C_7H_{16}/O_2/N_2$ in JSR doped with (50 and 500 ppm NO) and without NO at 10 atm, ϕ = 1.0, τ = 1.0 s. Solid lines: prediction without CH_3NO_2 chemistry, dashed lines: prediction with CH_3NO_2 chemistry. Left figure (50 ppm NO), right figure (500 ppm of NO)

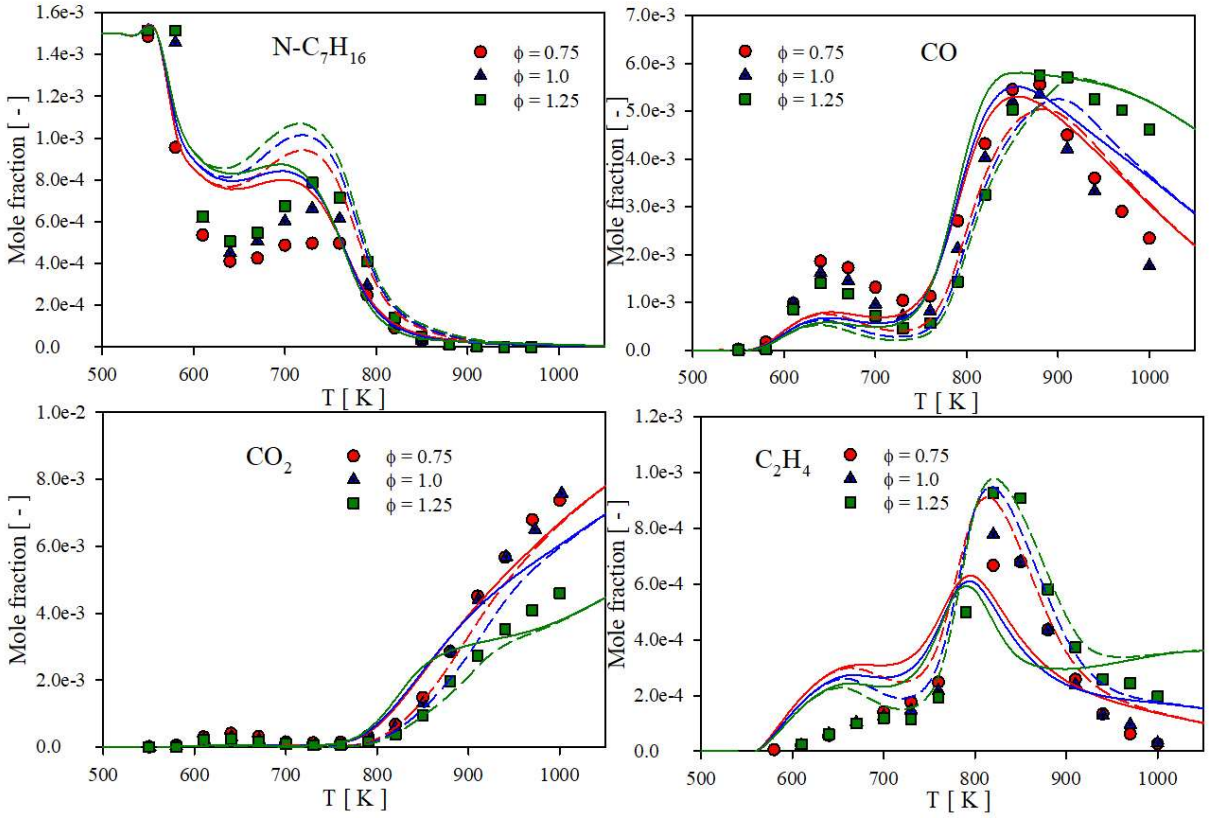

Figure S9: Oxidation of n-$C_7H_{16}/O_2/N_2$ in JSR doped with 50 ppm of NO at 10 atm, τ = 1.0 s and different ϕ. Symbols: measurements from [2], Solid lines: prediction without CH_3NO_2 chemistry, dashed lines: prediction with CH_3NO_2 chemistry.

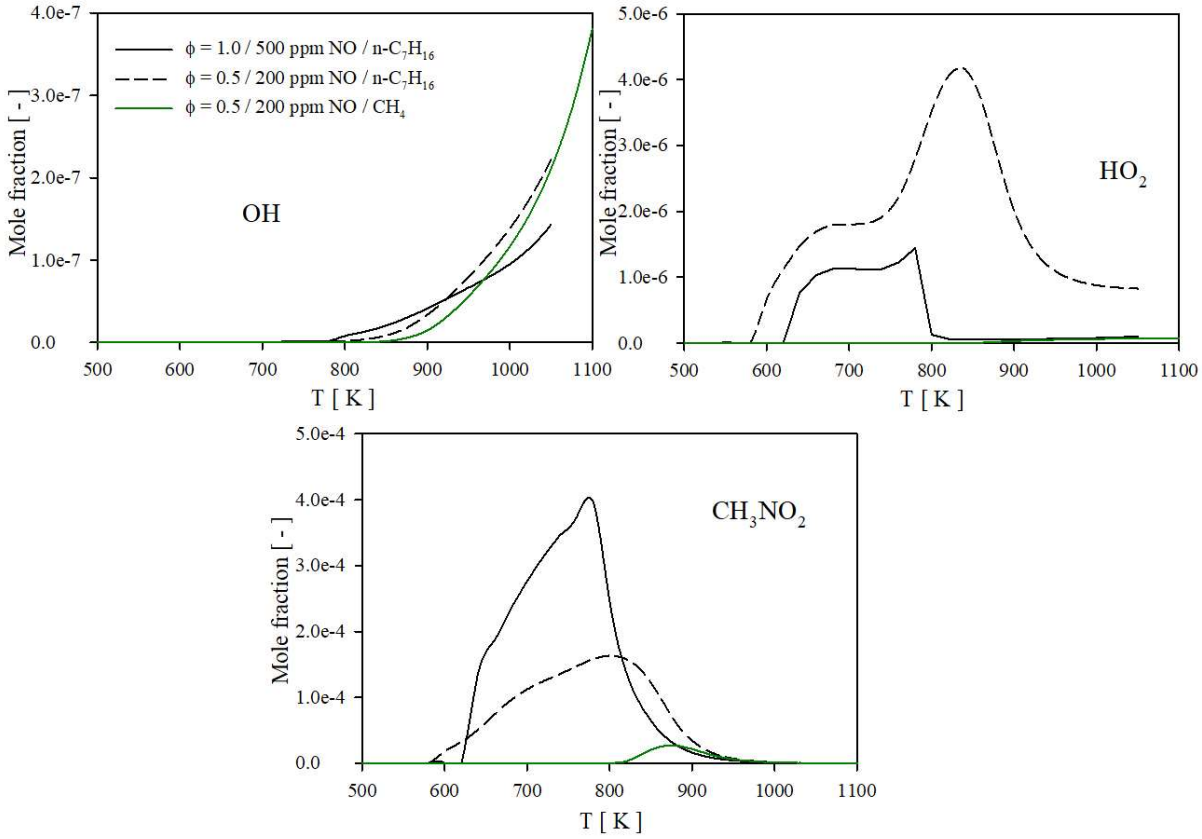

Figure S10: OH, HO_2 and CH_3NO_2 mole fraction profile comparison of n-heptane oxidation and methane oxidation in JSR. Solid lines: initial condition are same as in Figure 1 and 5, dashed lines: for n-heptane oxidation in JSR at ϕ = 0.5 and doped with 200 ppm of NO to have one to one comparison with methane.

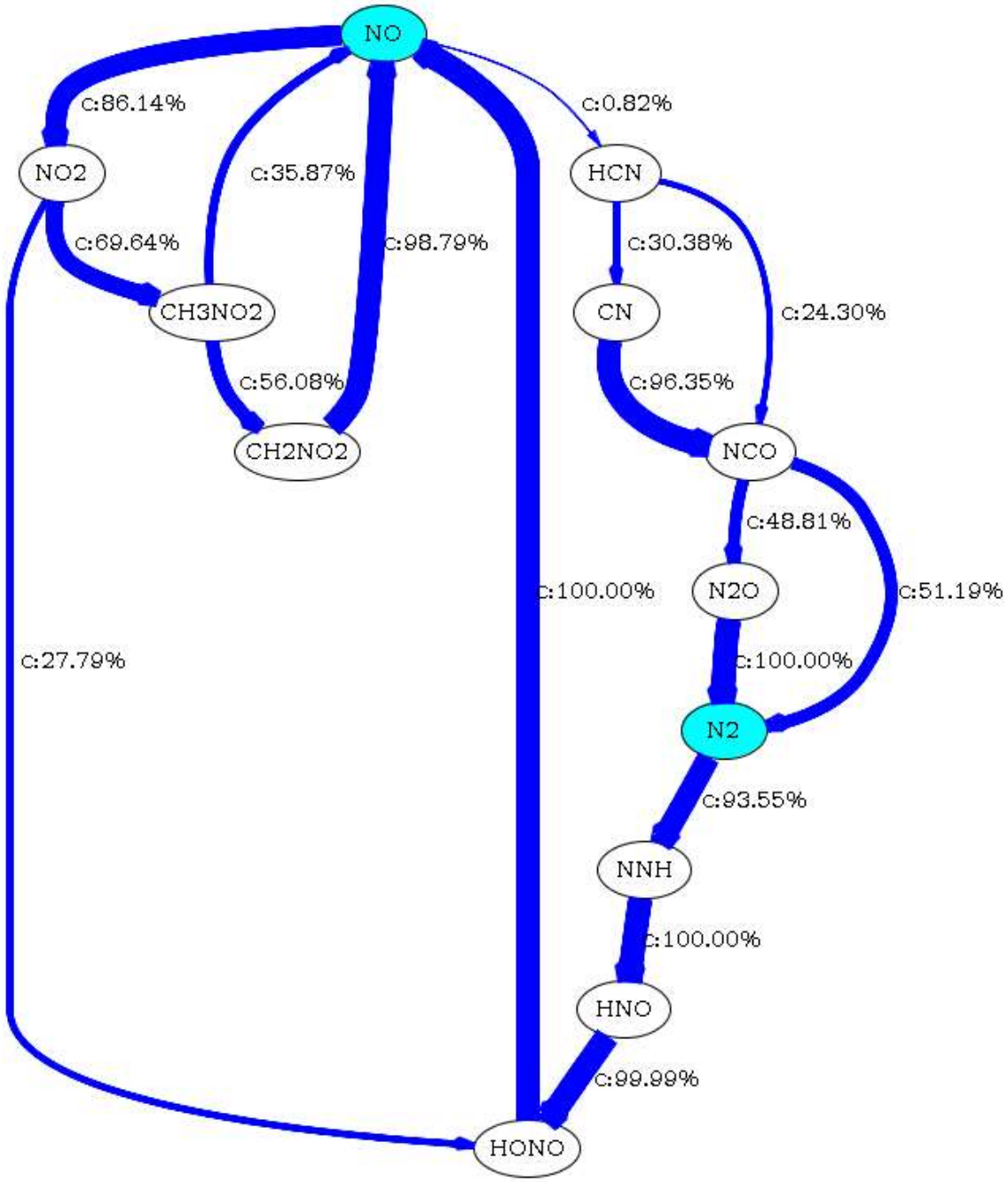

Figure S11: Reaction path analysis for CH_4 oxidation in JSR for the condition shown in Figure 1 (doped with NO) based on N-atom at 900 K.

References

[1] Y. Song, L. Marrodán, N. Vin, O. Herbinet, E. Assaf, C. Fittschen, A. Stagni, T. Faravelli, M.U. Alzueta, F. Battin-Leclerc, The sensitizing effects of NO 2 and NO on methane low temperature oxidation in a jet stirred reactor, Proc. Combust. Inst. 37 (2019) 667–675. doi:10.1016/j.proci.2018.06.115.

[2] G. Moréac, Experimental study and modelling of chemical interactions between gases residual and fresh gas in the homogeneous spontaneous ignition gasoline engines, PhD Thesis, University of Orléans, 2003. https://tel.archives-ouvertes.fr/tel-02961685/.