

Supplementary document

Experimental and Numerical Investigation of the Promoting Effect of a Cetane Booster in a Low-Octane Gasoline Fuel in a Rapid Compression Machine: a Study of 2-Ethylhexyl Nitrate

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Kinetic model validation

Experiments conducted in plug flow reactors

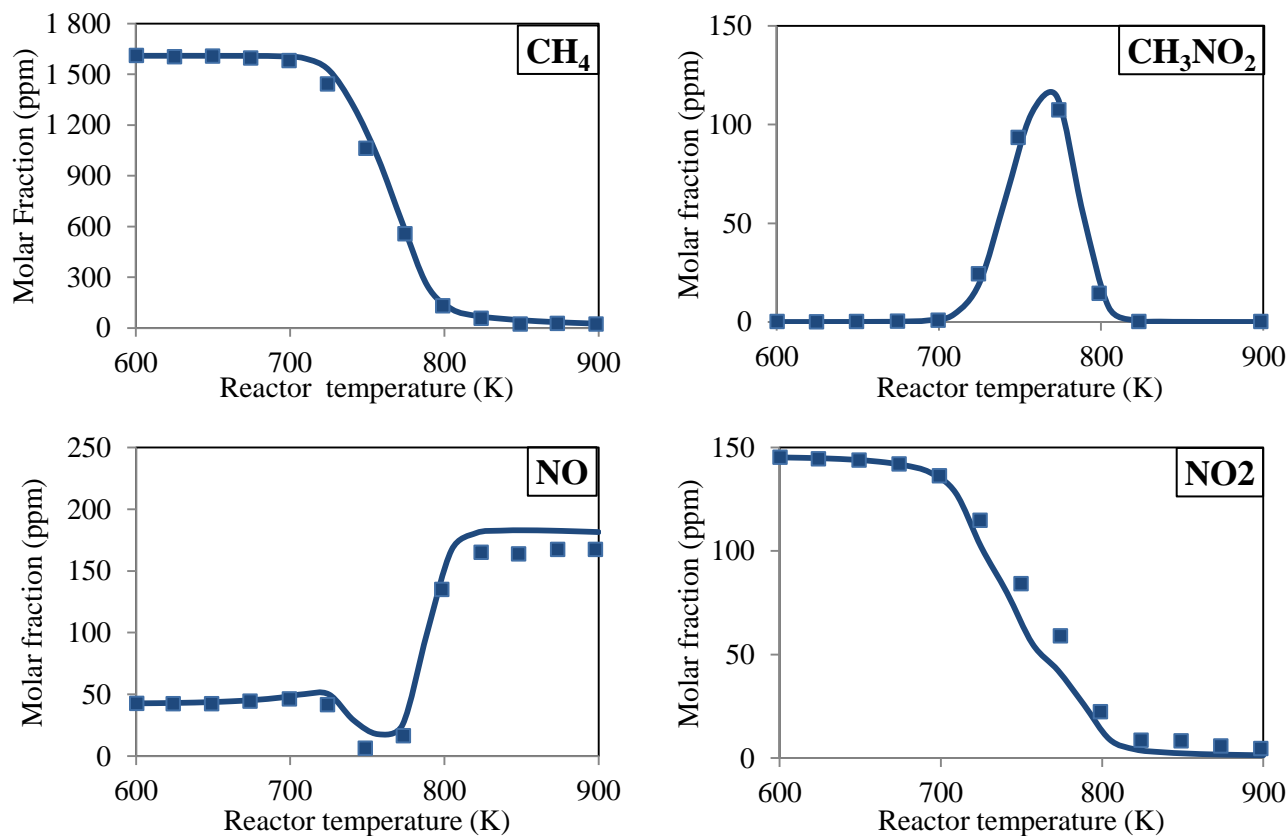


Figure S1. Species profiles of CH₄, CH₃NO₂, NO and NO₂ at 50 atm, $\Phi = 1.15$, from 500 to 900 K. Symbols: experimental results. Lines: simulations results. Initial fuel mixture: CH₄ (1610 ppm)/ NO (43 ppm)/ NO₂ (145 ppm)/ O₂ (2798 ppm)/ N₂ (99.54% mol.). Experiments conducted by Rasmussen et al.[1].

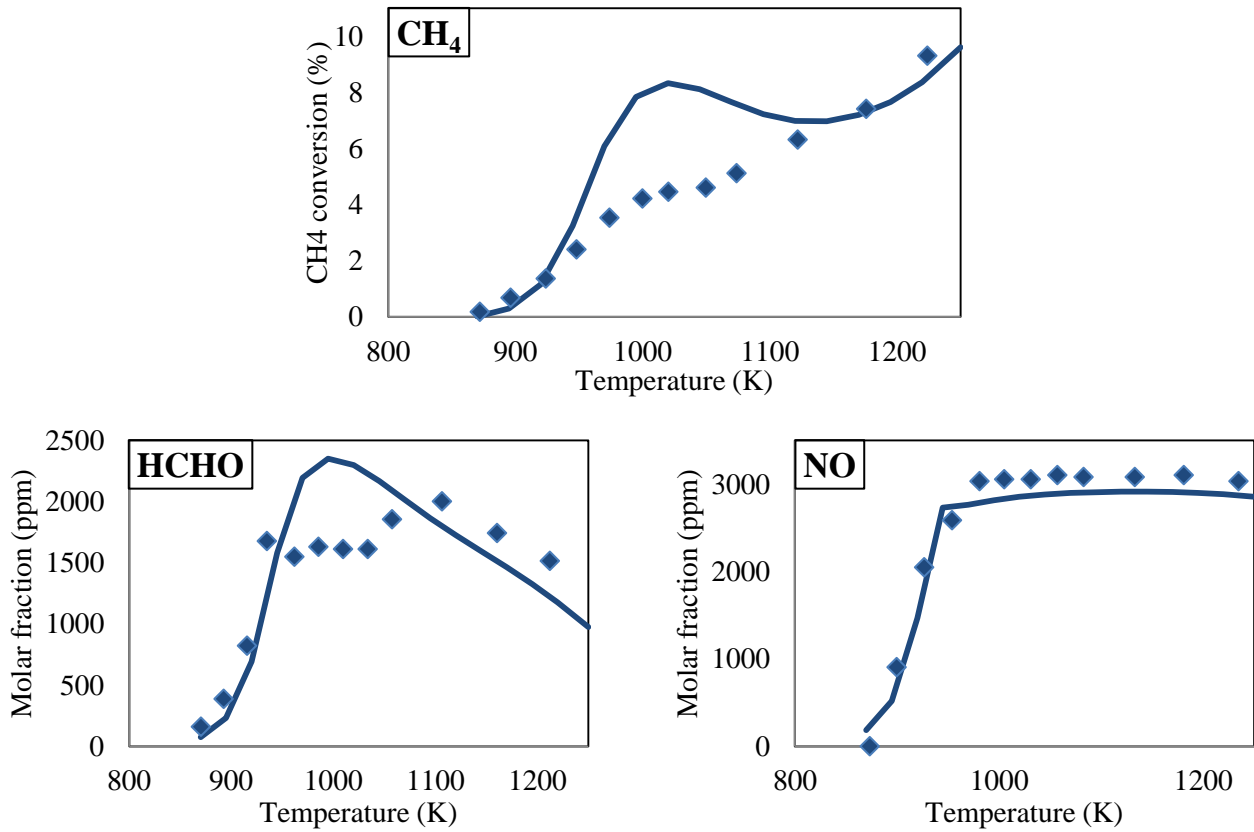


Figure S2. CH₄ conversion and concentrations of HCHO and NO as a function of reactor temperature. Experimental conditions: 2 bar, $\Phi = 4$. Symbols: experimental results. Lines: simulations results. Initial fuel mixture: CH₄ (6667 ppm)/ NO₂ (300 ppm)/ O₂ (3.3% mol.)/ Ar (89.7% mol.). Experiments conducted by Zhang et al.[2]

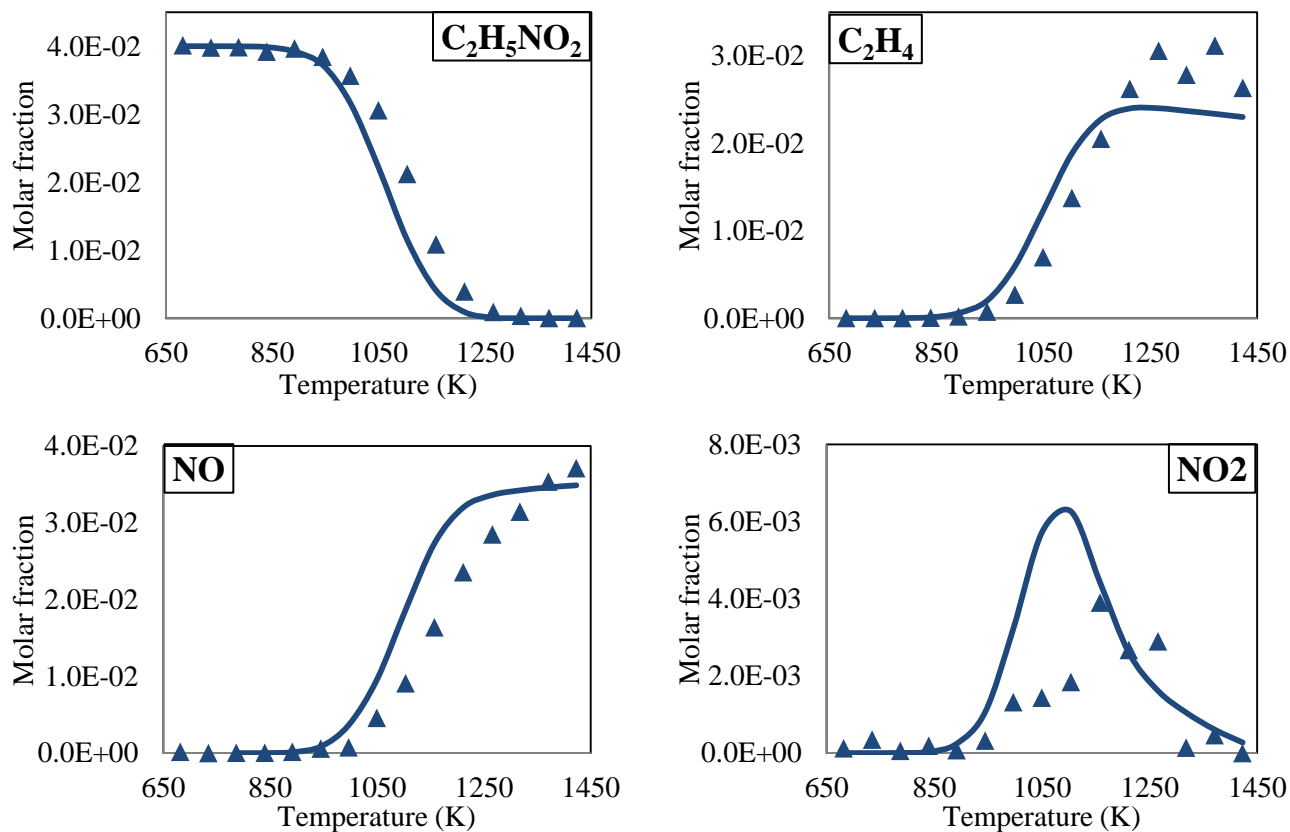


Figure S3. Species profiles of $C_2H_5NO_2$, C_2H_4 , NO and NO_2 as a function of reactor temperature during $C_2H_5NO_2$ pyrolysis. Experimental conditions: 5 torr, from 650 to 1450 K. Symbols: experimental results. Lines: simulations results. Initial fuel mixture: $C_2H_5NO_2$ (4% mol.)/ Ar (96% mol.) Experiments conducted by Zhang et al.[3].

Experiments conducted in perfectly stirred reactors

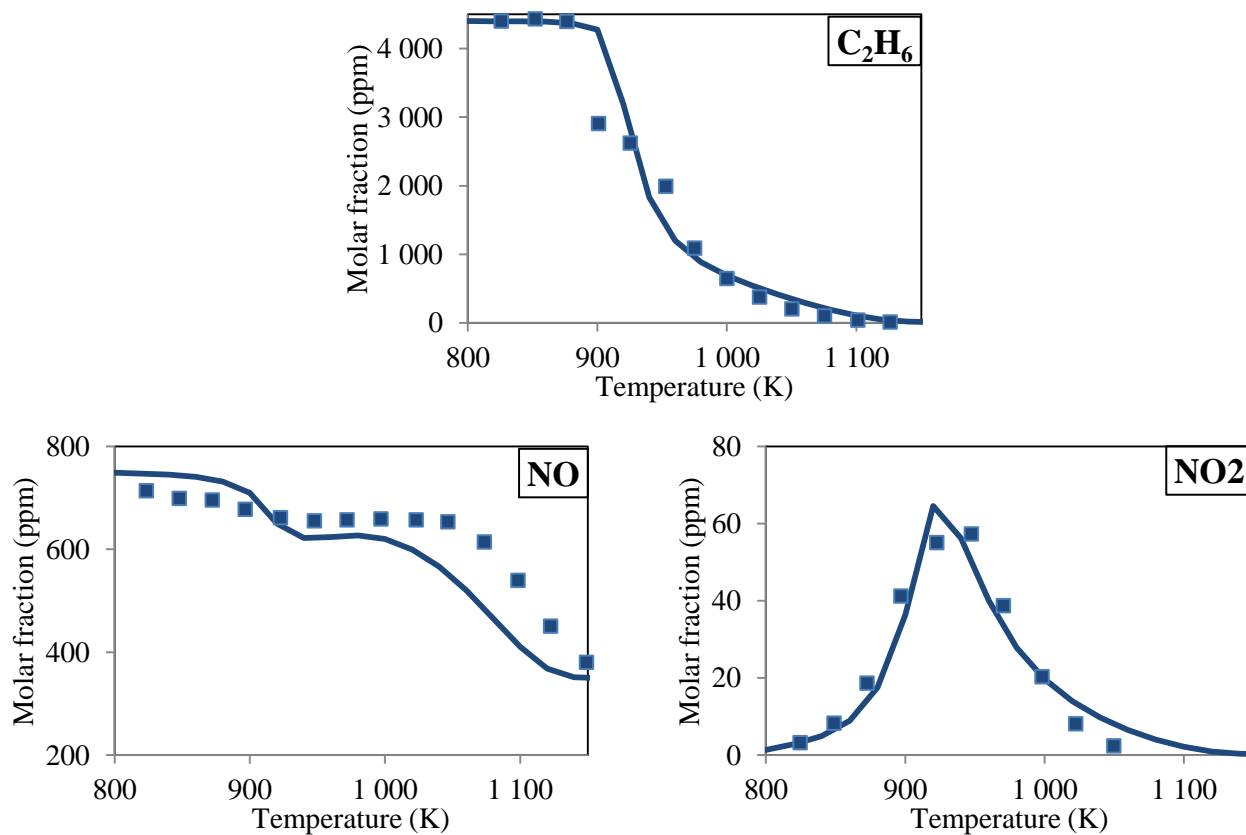


Figure S4. Species profiles of C₂H₆, NO, NO₂ as a function of reactor temperature. Experimental conditions: 1 atm, $\Phi = 1$, residence time: 0.13 s. Symbols: experimental results. Lines: simulations results. Initial fuel mixture: C₂H₆ (4400 ppm)/ NO (750 ppm)/ O₂ (1.54% mol.)/ N₂ (97.95% mol.) . Experiments conducted by Dagaut et al.[4].

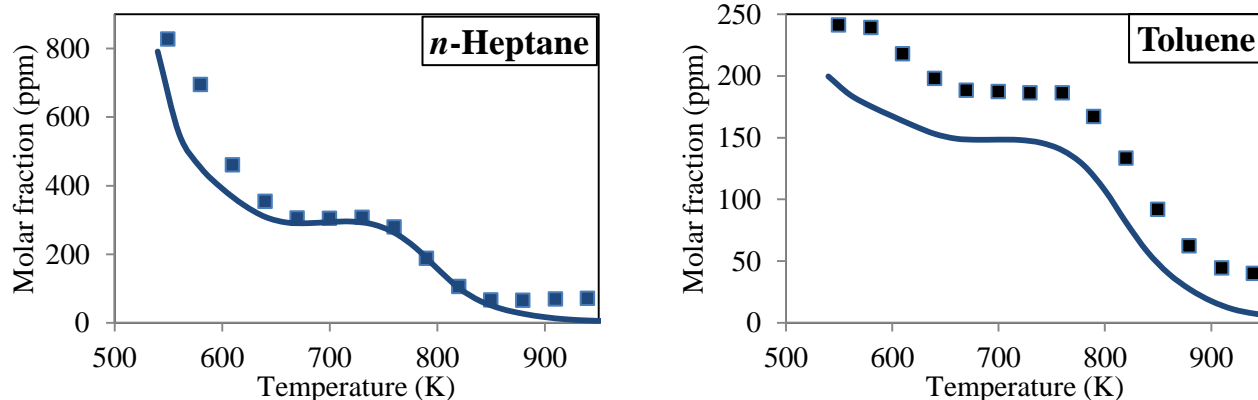


Figure S5. Species profiles of *n*-heptane and toluene as a function of reactor temperature. Experimental conditions: 10 atm, $\Phi = 0.2$, residence time: 0.5 s. Symbols: experimental results. Lines: simulations results. Initial fuel mixture: *n*-heptane (800 ppm)/ toluene (200 ppm)/ NO (50 ppm)/ O₂ (5.3% mol.)/ N₂ (94.6% mol.) . Experiments conducted by Dubreuil et al.[5].

Experiments conducted in shock tubes

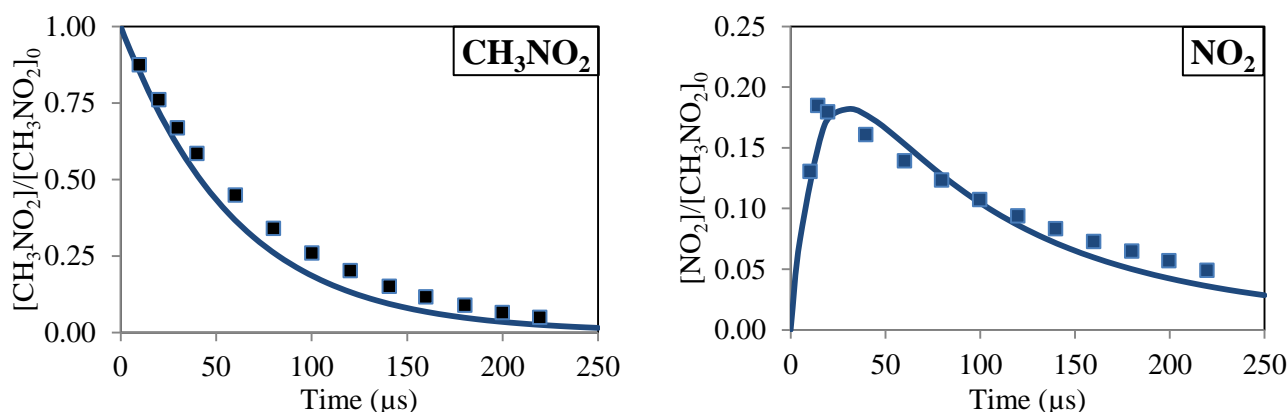


Figure S6. Species profiles of CH₃NO₂ and NO₂ as a function of time. Experimental conditions: 5.95 atm, T = 1180 K. Symbols: experimental results. Lines: simulations results. Initial fuel mixture: 370 ppm CH₃NO₂ in Argon. Experiments conducted by Glänzer and Troe [6].

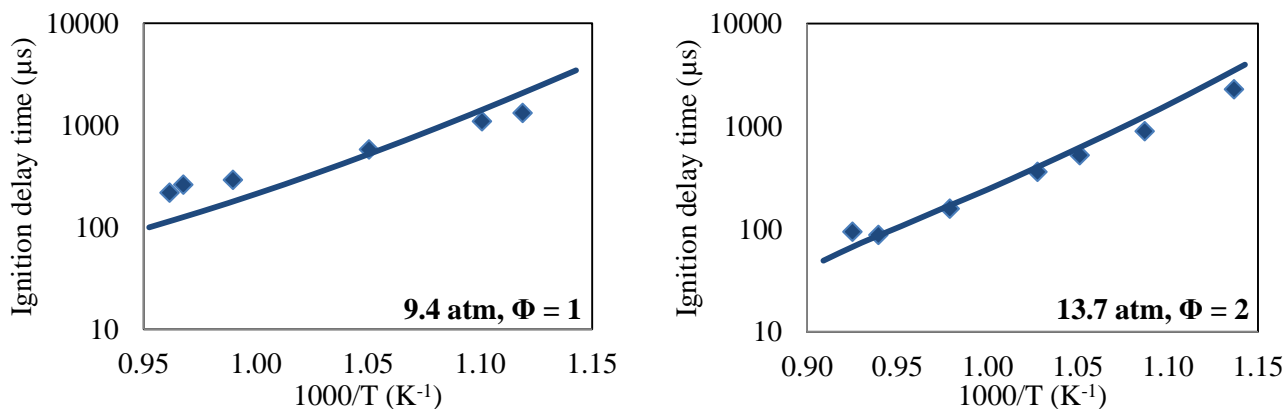


Figure S7. Ignition delay time of nitromethane (CH_3NO_2) at different pressures and equivalence ratios. Symbols: experimental results. Lines: simulations results.. Experiments conducted by Mathieu et al.[7].

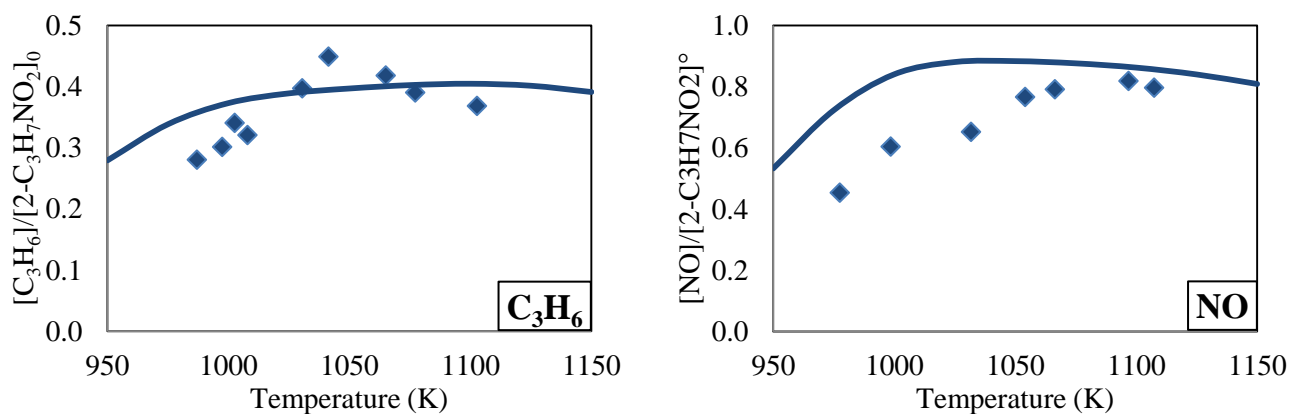


Figure S8. Species profiles of C_3H_6 and NO as a function of temperature. Experimental conditions: 5 atm, reaction time: 1.3 ms. Symbols: experimental results. Lines: simulations results. Initial fuel mixture: 6500 ppm 2-nitropropane ($2\text{-C}_3\text{H}_7\text{NO}_2$) in Argon. Experiments conducted by Zhang et al.[8].

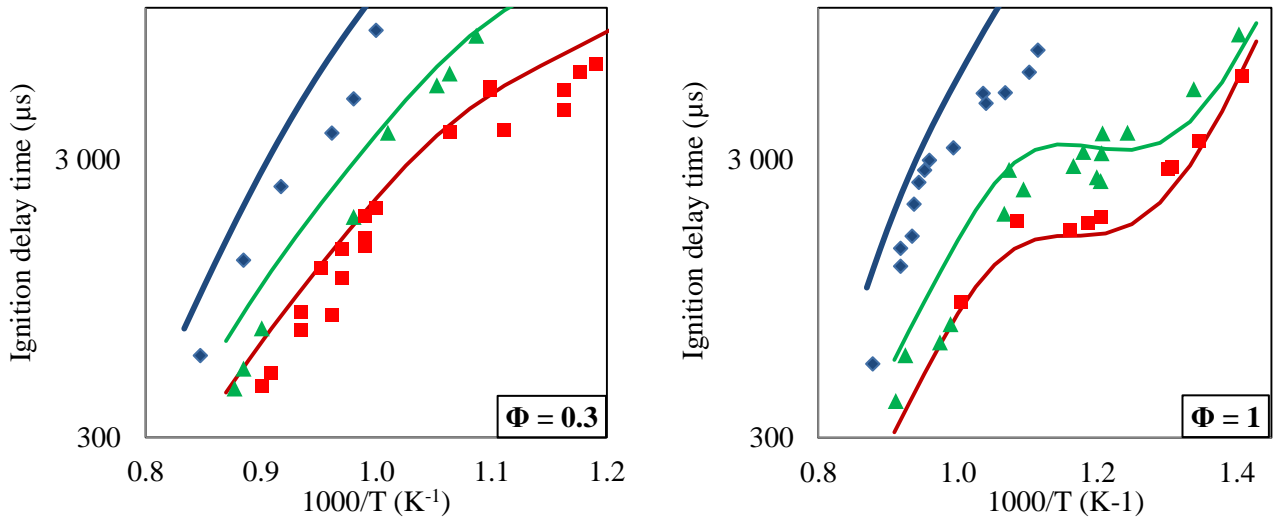


Figure S9. Ignition delay time of the mixture of *n*-heptane (35% vol.) and toluene (65% vol.) in air ($\Phi = 0.3$ and 1) at different pressures: 10 bar (blue), 30 bar (green) and 50 bar (red). Symbols: experimental results. Lines: simulations results. Experiments conducted by Herzler et al.[9].

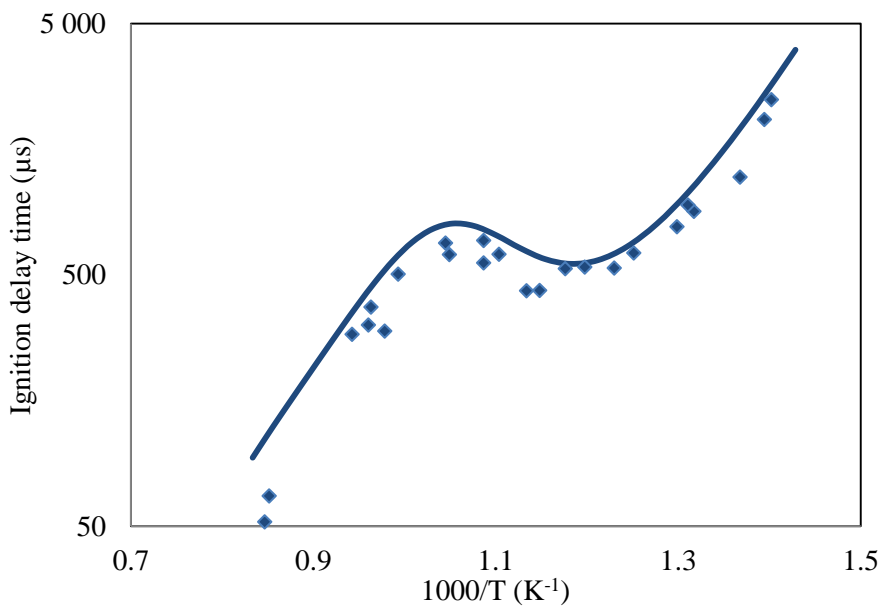


Figure S10. Ignition delay time of the mixture of *n*-heptane (90% vol.) and toluene (10% vol.) in air ($\Phi = 1$) at 40 bar. Symbols: experimental results. Lines: simulations results. Experiments conducted by Hartmann et al.[10].

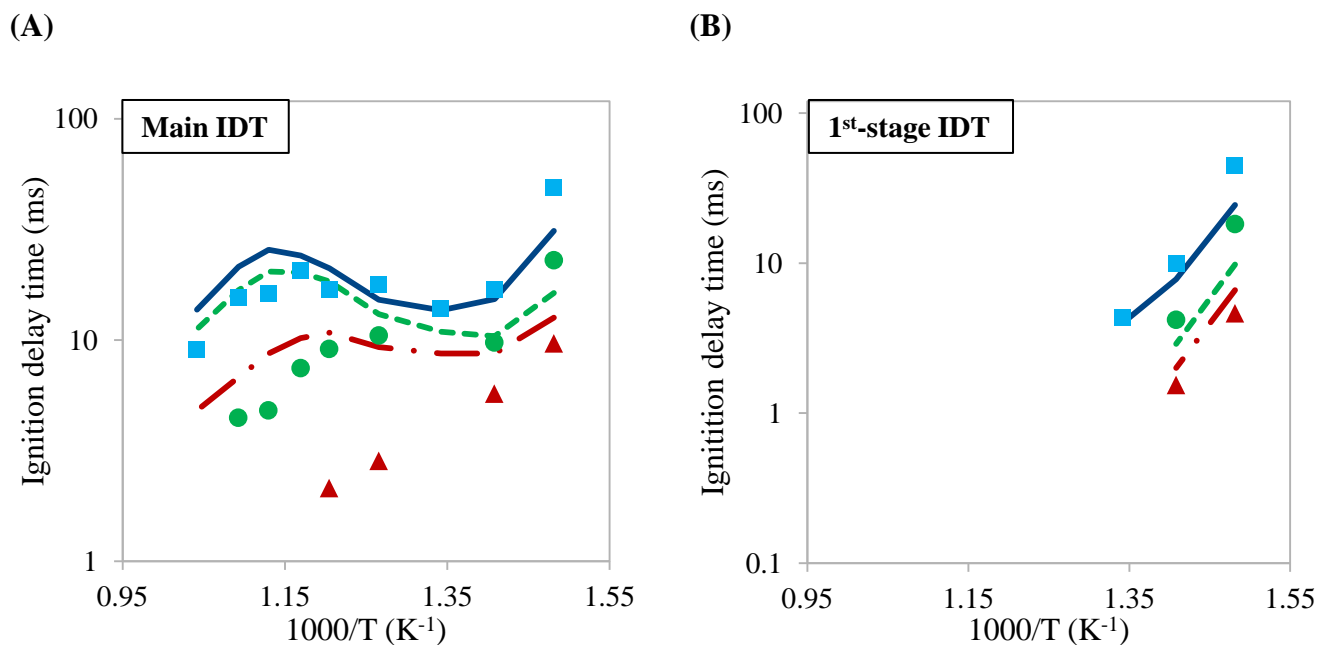


Figure S11. Measured and simulated 1st-stage and main IDT of the neat and doped fuels. The “frozen chemistry” simulation method is employed. Symbols refer to experimental data and lines are used to illustrate modeling work. The neat surrogate fuel results are illustrated with solid lines and square symbols. Doped fuels with 0.1% EHN is presented with dashed lines and circle symbols and 1% EHN with dash-dotted lines and triangle symbols. (A) Main IDT, (B) 1st-stage IDT.

References

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