Table 1. Physical properties of n-heptane and 1-heptene at 20°C and 1atm.

	n-heptane	1-heptene
Critical temperature, °C	540	537
Boiling point, °C	98.4	93.6
Density, kg/m^3	690	697
Vapor pressure, kPa	4.7	7.9
Liquid viscosity, mPa.s	0.376	0.349

Table 2. Experimental conditions for non-reacting and reacting n-heptane sprays.

Temperature, K	800 – 1300 (reacting) 1000 (non-reacting & base case)
O2 volume fraction, %	8 – 21 (reacting) 21 (base case) 0 (non-reacting case)
Density, kg/m^3	14.8
Injection pressure, MPa	150
Injection duration, ms	6.8
Injection mass, mg	17.8
Nozzle diameter, mm	0.1
Discharge coefficient (C_d)	0.8
Area contraction coefficient (C_a)	0.86

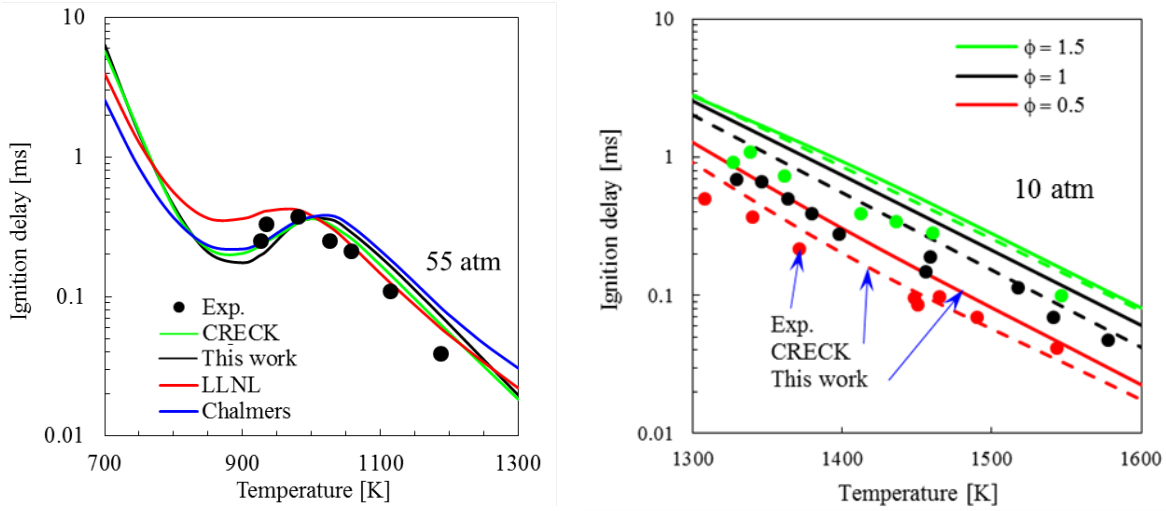


Fig 1: Predicted and measured ignition delays for n-heptane/air at p = 55 atm and ϕ = 1 (a), and for 1-heptene/air mixtures (b) at p = 10 atm, and three equivalence ratios, ϕ = 1.5, [C_7H_{14}] =1248 ppm, ϕ = 1, [C_7H_{14}] = 873.3 ppm, and ϕ = 0.5, [C_7H_{14}] = 447.6 ppm. Ignition delay is defined as the time for OH mole fraction to attain 50% of the peak value. Solid and dashed lines in Fig. 1b indicate simulation results with the reduced and detailed CRECK mechanisms, respectively.

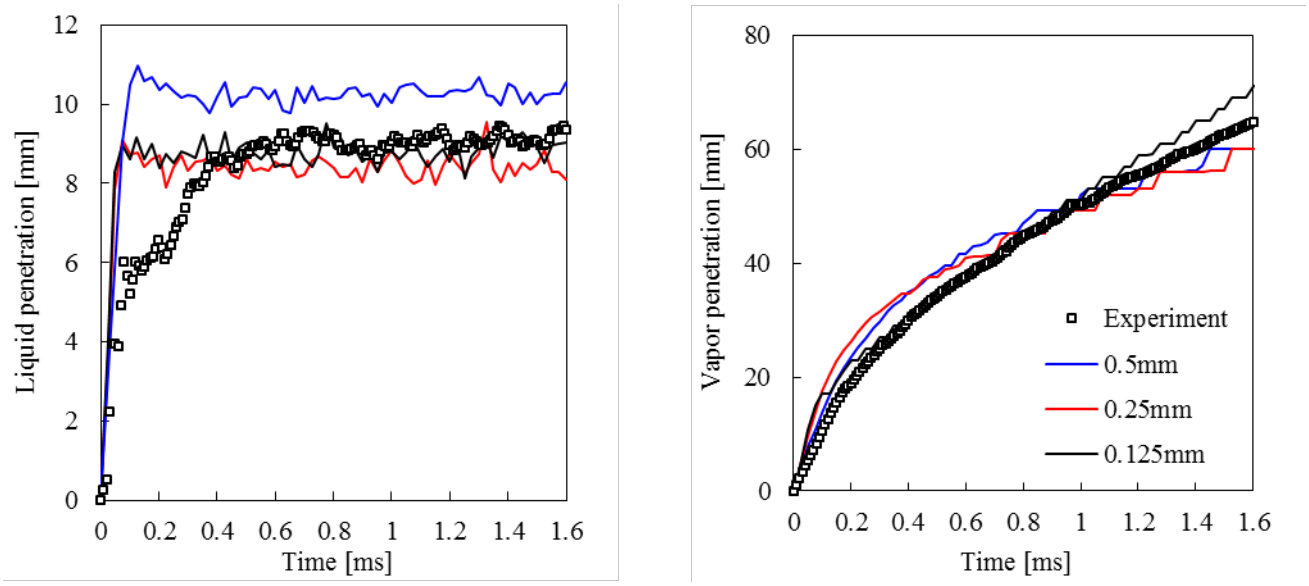


Fig 2: Measured and predicted liquid penetration (a) and vapor penetration (b) distances for n-heptane non-reacting spray. Predictions are shown for three grid sizes of 0.5mm, 0.25mm and 0.125mm.

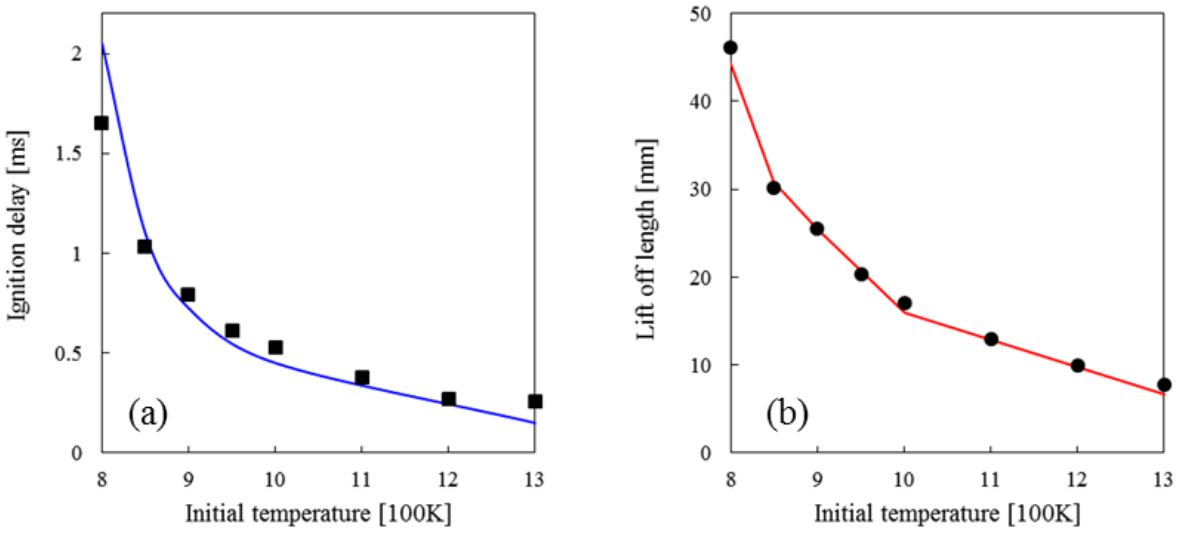


Fig 3: Measured (symbols) and predicted ignition delay (a) and flame LOL (b) plotted versus initial temperature.

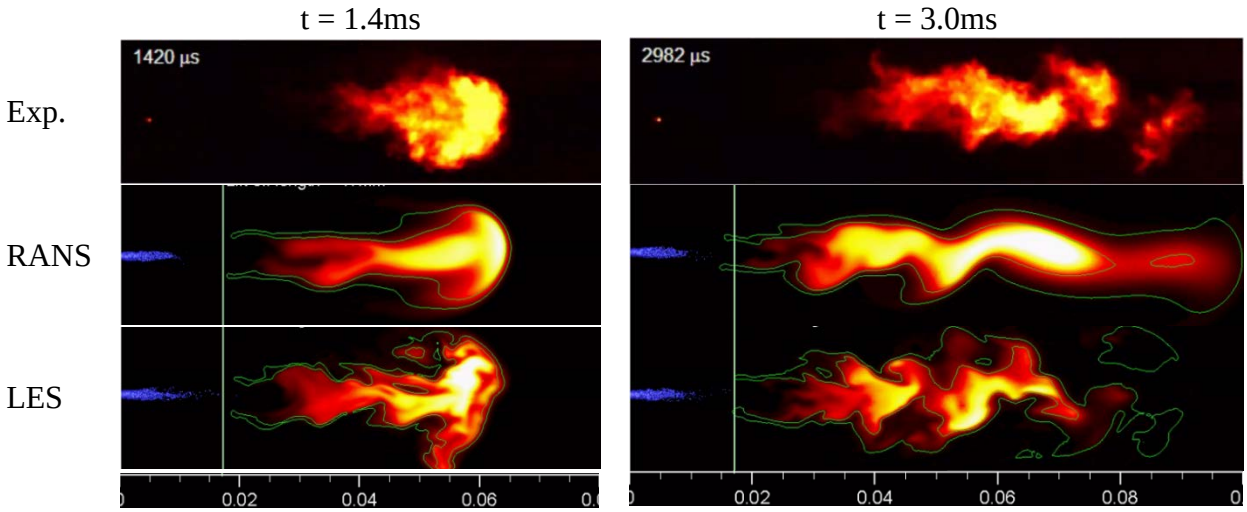


Fig 4: Comparison of measured soot luminosity images with the predicted soot mass fraction contours for n-heptane reacting spray for ambient temperature=1000K, density=14.8kg/m^3, O_2 mole fraction=0.21, and injection pressure=150MPa. Solid vertical lines at 0.017m in the computed images indicate the measured flame LOL. Green contour line represents the predicted OH mass fraction corresponding to 2% of the peak value.

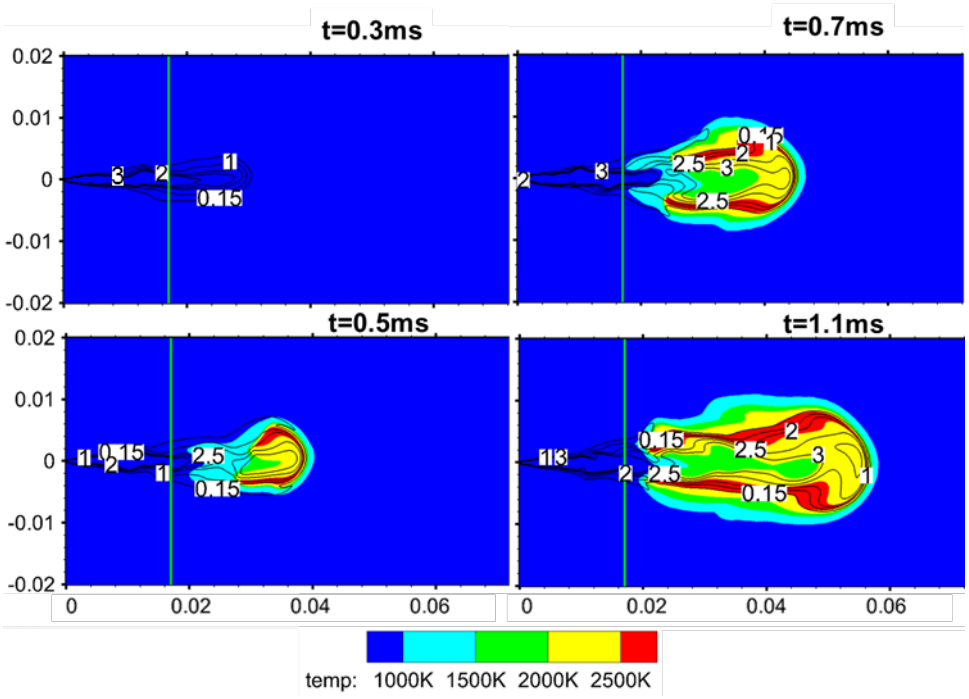


Fig 5: Mixture fraction and temperature contours at different times (after start of injection) showing the temporal evolution of n-heptane spray flame. Colors indicate temperatures 1000-2500K. Contour lines represent mixture fraction or equivalence ratio between 0.15-3. Initial temperature=1000K. Dimensions are in m.

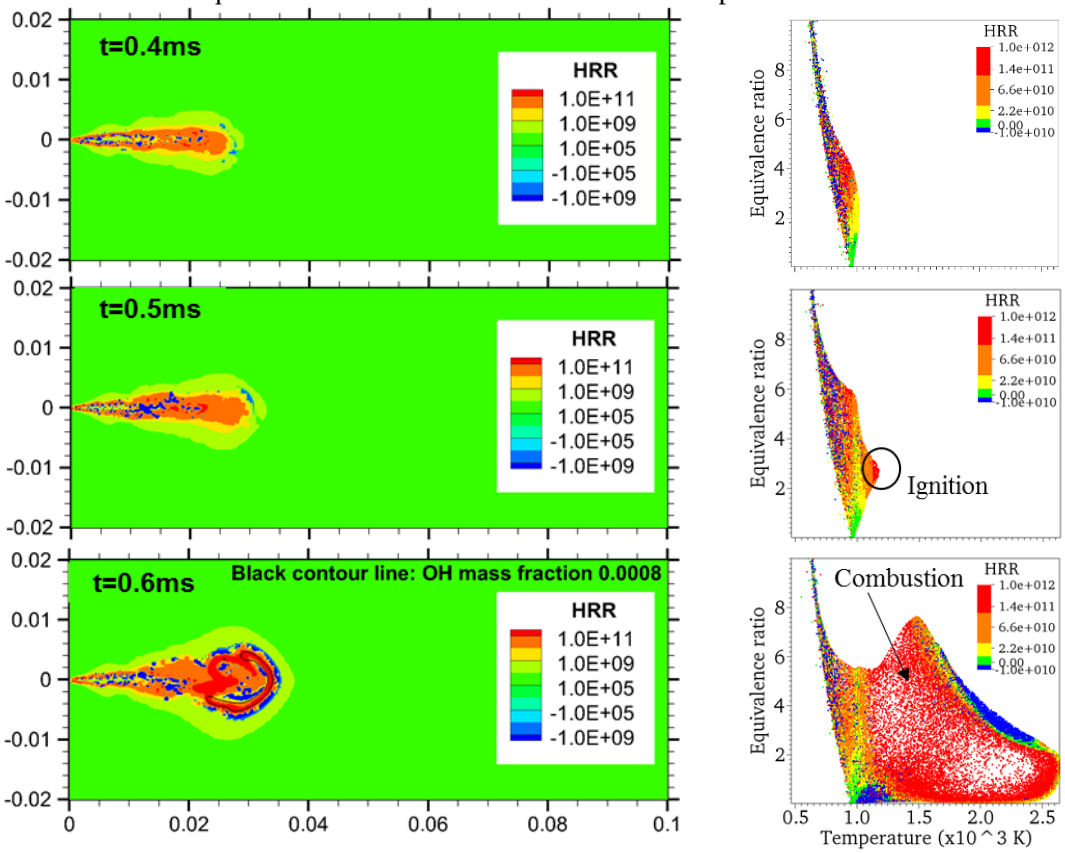


Fig 6: Heat release rate (J/s-m^3) contours (left) and scatter plots in ϕ-T space (right) at different times after SOI. Heat release rates between -1x10^9 to 1x10^{11} for contours and between -1x10^{10} to 1x10^{12} for scatter plots.

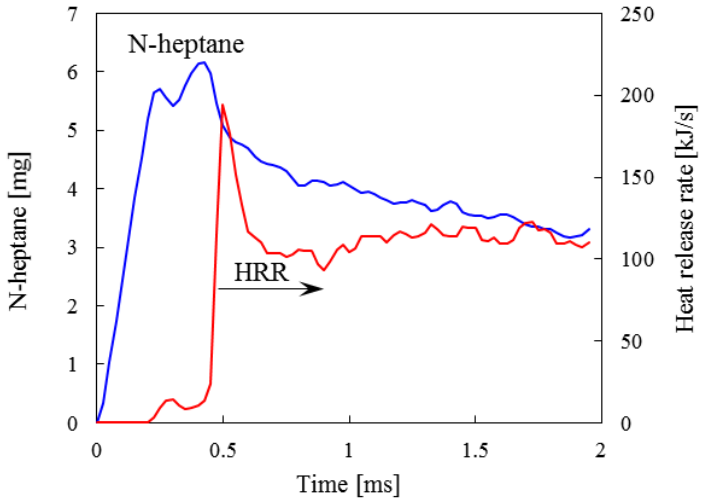


Fig 7: Integrated n-heptane vapor mass and heat release rate profiles with respect to time.

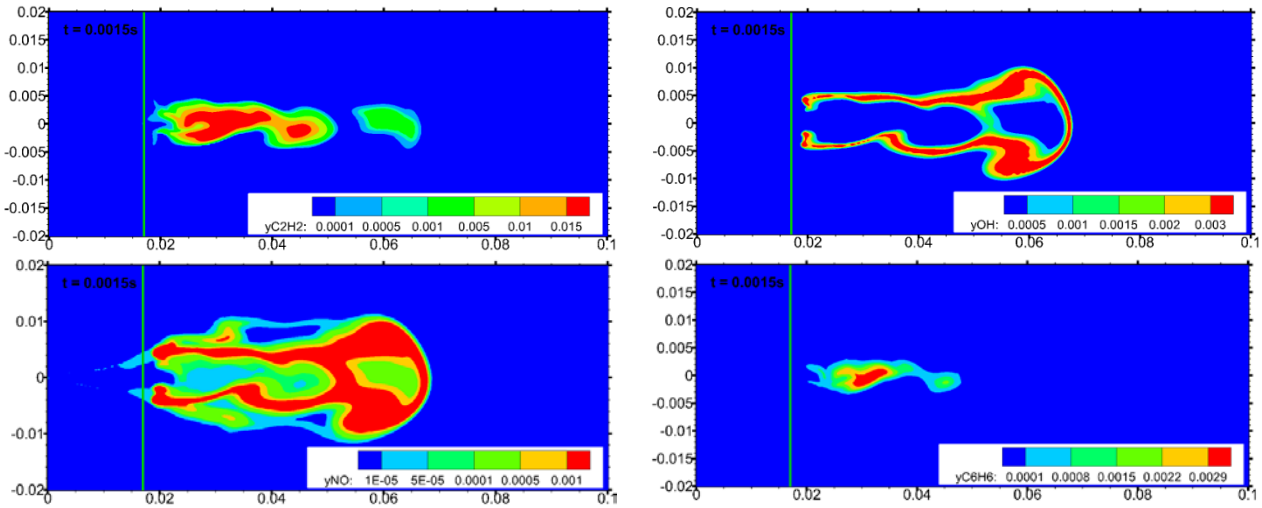
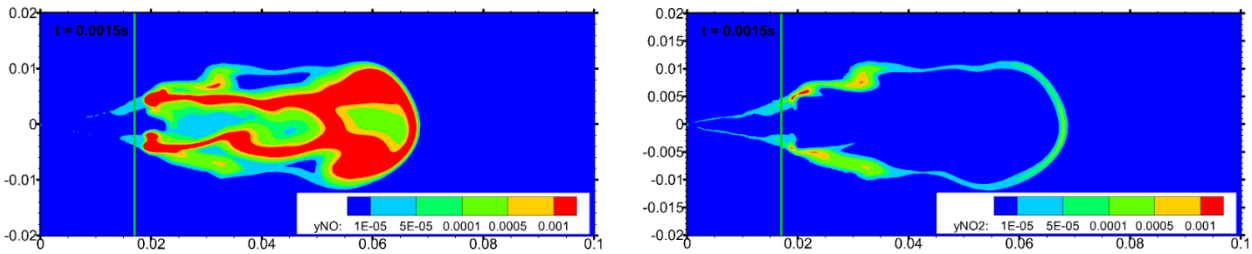
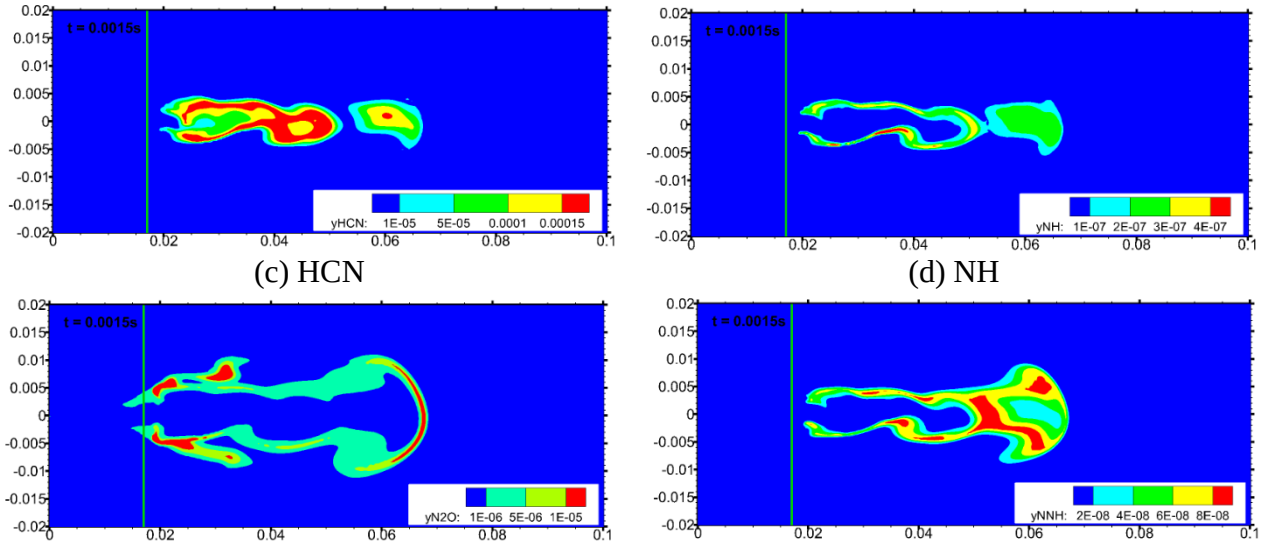


Fig 8: C_2H_2, OH, NO, and C_6H_6 mass fraction contours in n-heptane spray flame at t=0.0015s.



(a) NO (b) NO_2



(c) HCN (d) NH

(e) N_2O (f) NNH

Fig 9: Mass fraction contours for NO, NO_2, HCN NH, N_2O, and NNH at 0.0015s in the constant volume reactor for n-heptane spray flame. Initial ambient temperature=1000K.

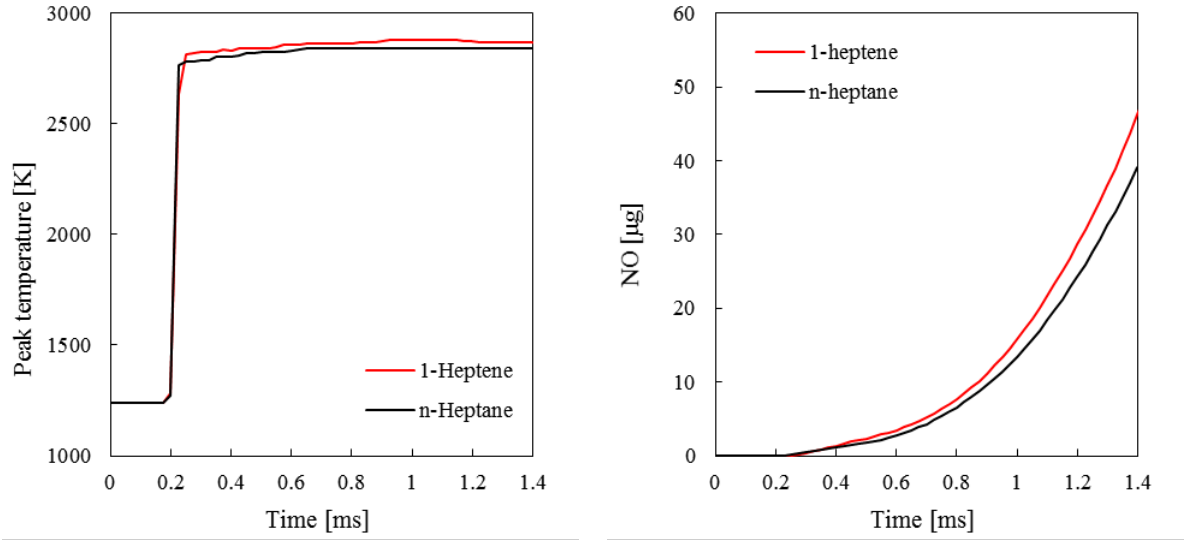


Fig 10: Peak temperature and total NO mass versus time for n-heptane (black) and 1-heptane (red) spray flames. Initial temperature is 1300K.

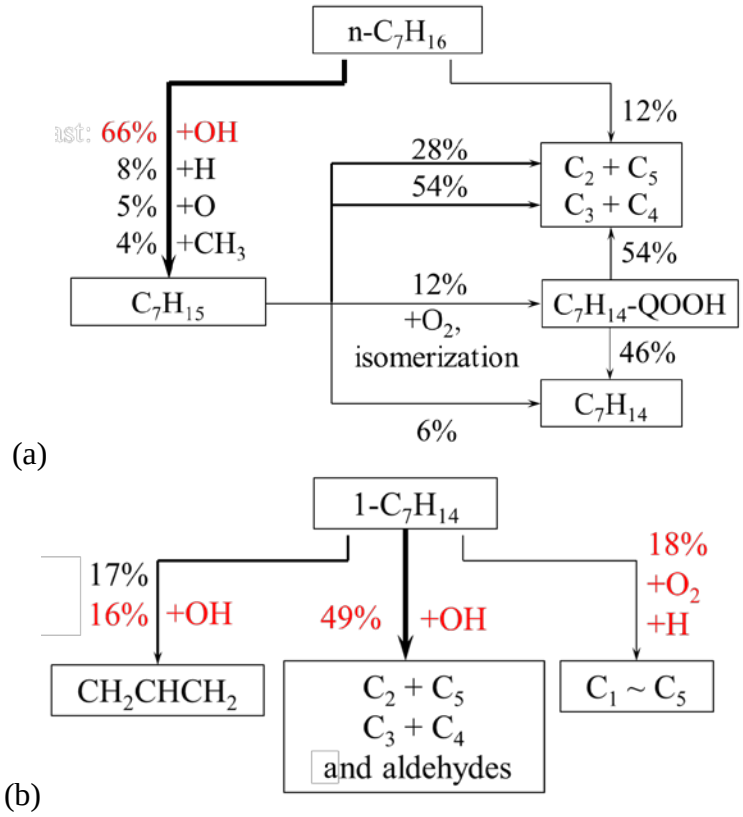


Fig 11: Dominant reaction paths for n-heptane (a) and 1-heptene (b) during ignition. Simulations are performed in a well-stirred reactor with initial T=1300K, p=55atm and ϕ=1. The red color indicates more dominant reactions. Percentage implies the relative amount of a species that is consumed though a given reaction. For example, in Fig. a, 66% of n-C_7H_{16} is consumed through its reaction with OH to form C_7H_{15}.

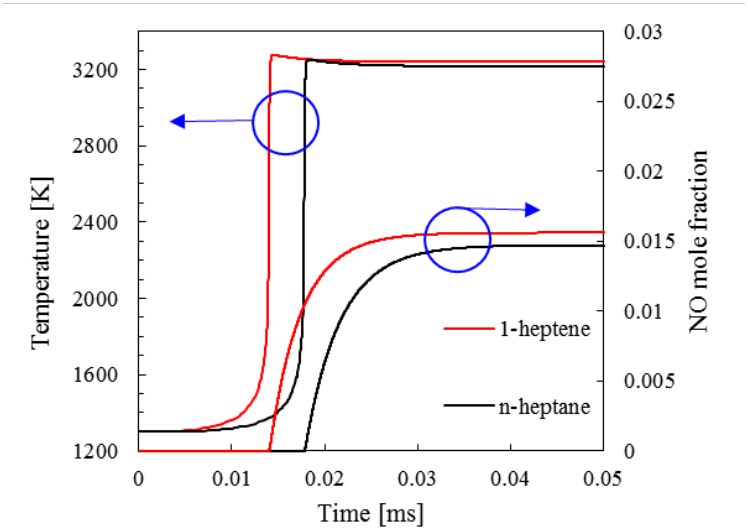


Fig 12: Temporal profiles of temperature and NO mole fraction for well-stirred reactor simulations with n-heptane and 1-heptene at initial T=1300K, p=55atm and ϕ=1.

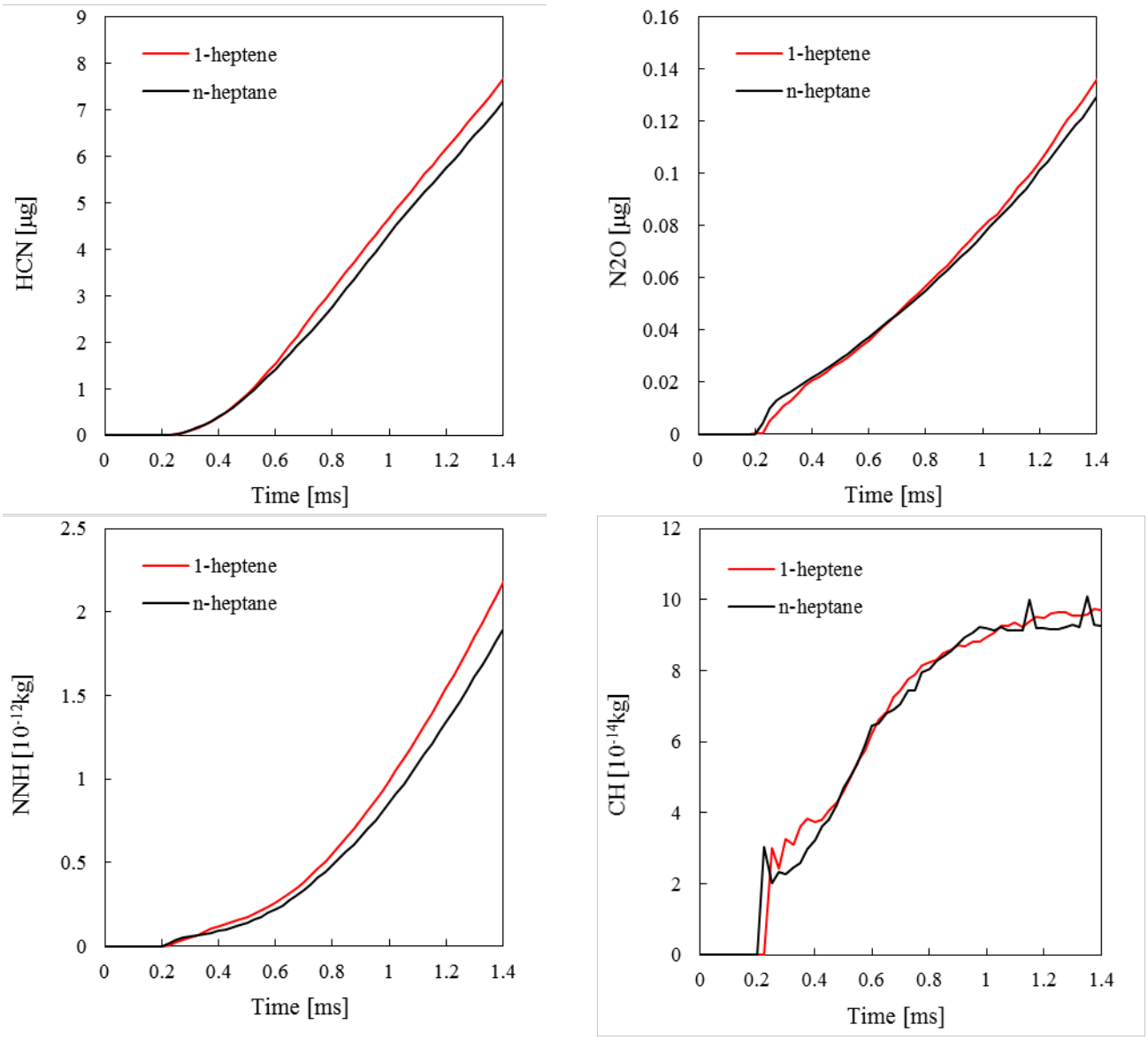


Fig 13: Total amounts of HCN, N_2O, NNH and CH species in n-heptane and 1-heptane flames. Initial temperature is 1300K.

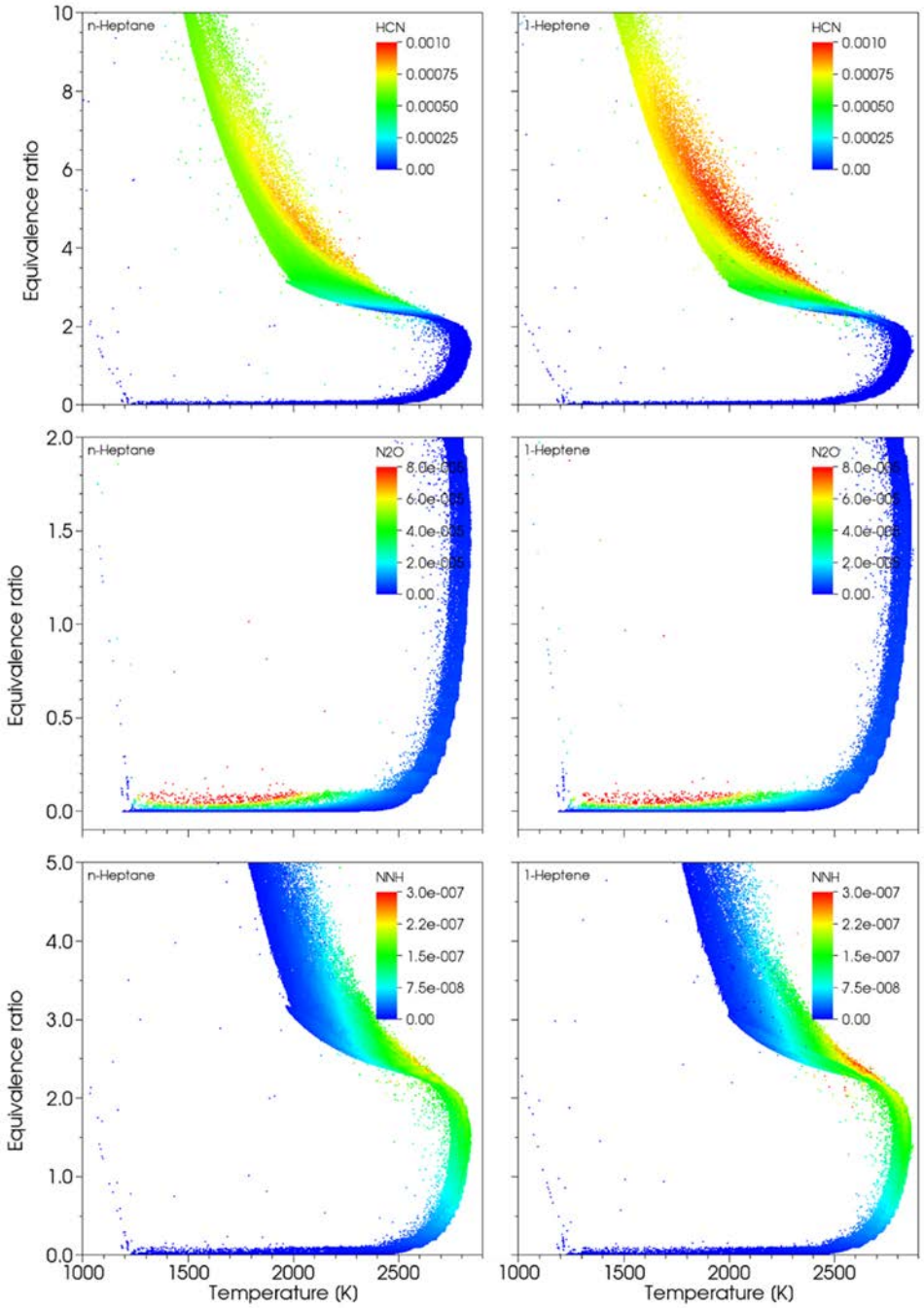


Fig 14: Scatter plots of HCN, N_2O and NNH in ϕ-T space for the n-heptane (left) and 1-heptene (right) flames at 1.4ms.

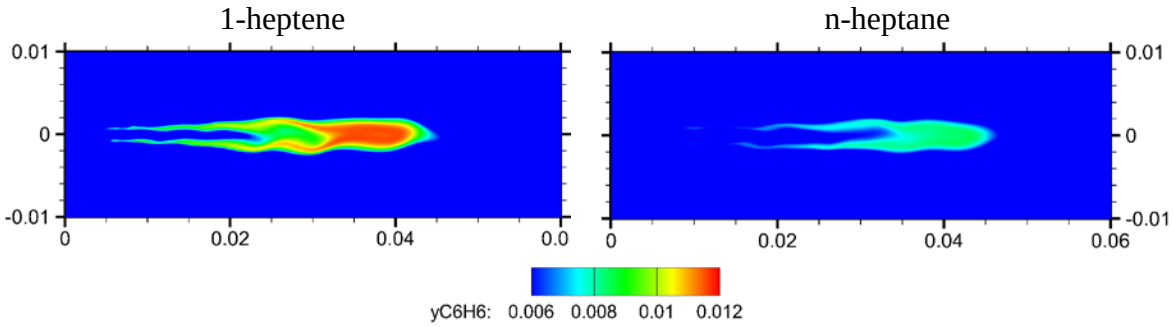


Fig 15: Benzene mass fraction contours for 1-heptene and n-heptane flames at 1.4ms. Mass fractions are between 0.006 and 0.012. Dimensions are in m.

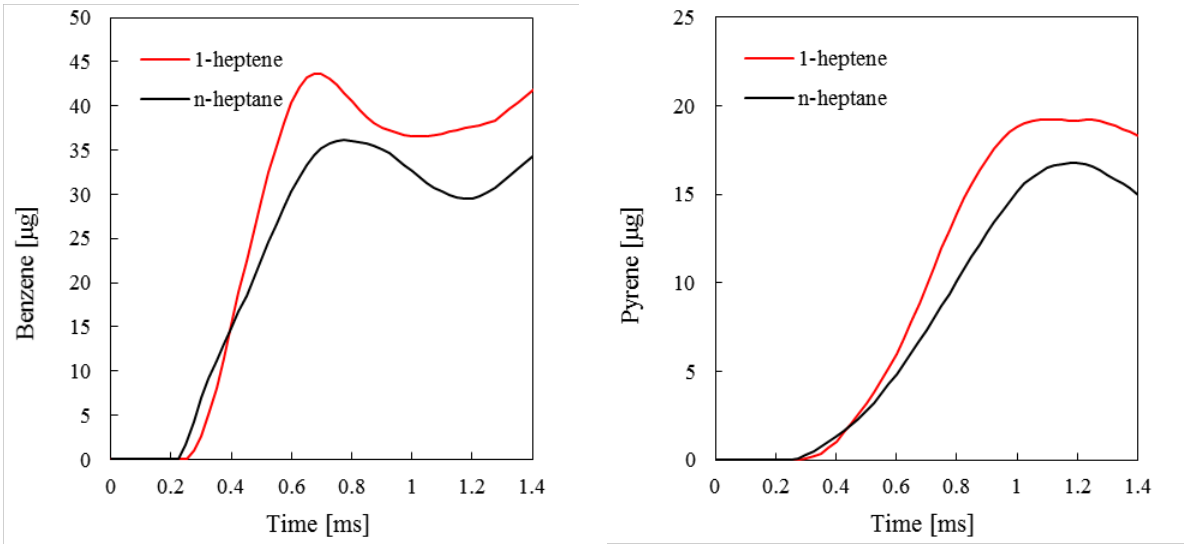
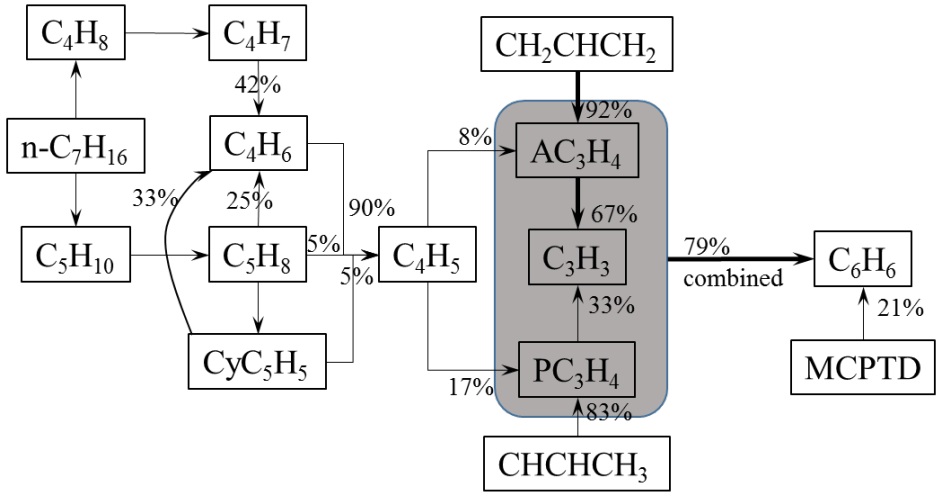
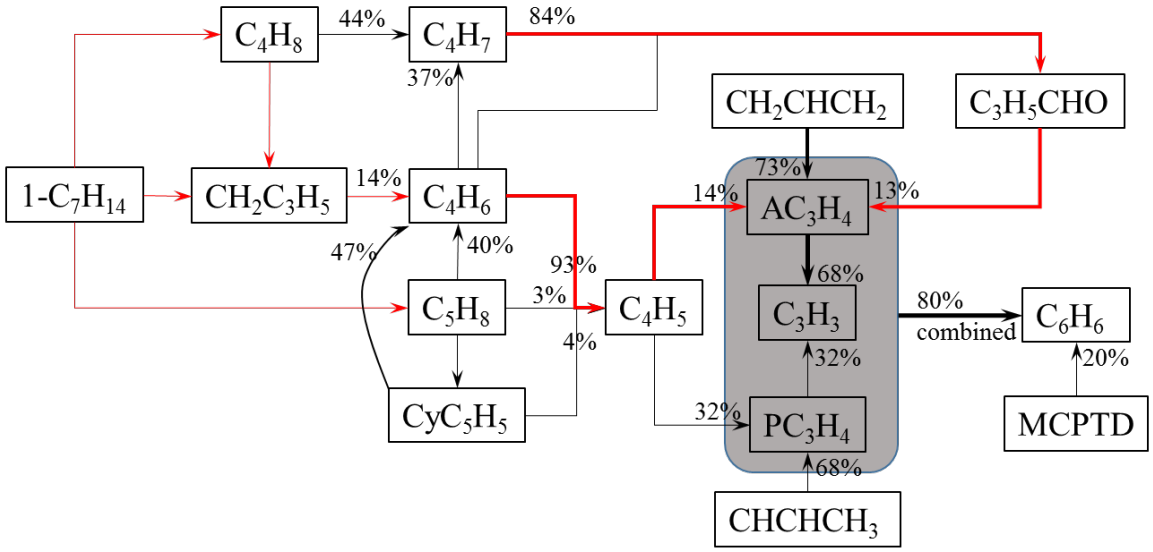


Fig 16: Integrated mass of benzene and pyrene for n-heptane (black) and 1-heptane (red) flames. Initial temperature is 1300K.



(a): n-Heptane



(b): 1-Heptene

Fig. 17: Dominant reaction paths for benzene formation for n-heptane (a) and 1-heptene (b). Simulations are performed in a well-stirred reactor with initial T=1300K, p=55atm and ϕ=1. The effect of double bond in 1-heptene on the various reactions are indicated by the red color. Also AC_3H_4: allene; PC_3H_4: propyne; MCPTD: methyl-cyclo-pentadiene. Percentage implies the relative amount of a species formed though a given reaction. For example, in Fig. a, 79% of C_6H_6 is formed through the combined reactions between C_3 species.

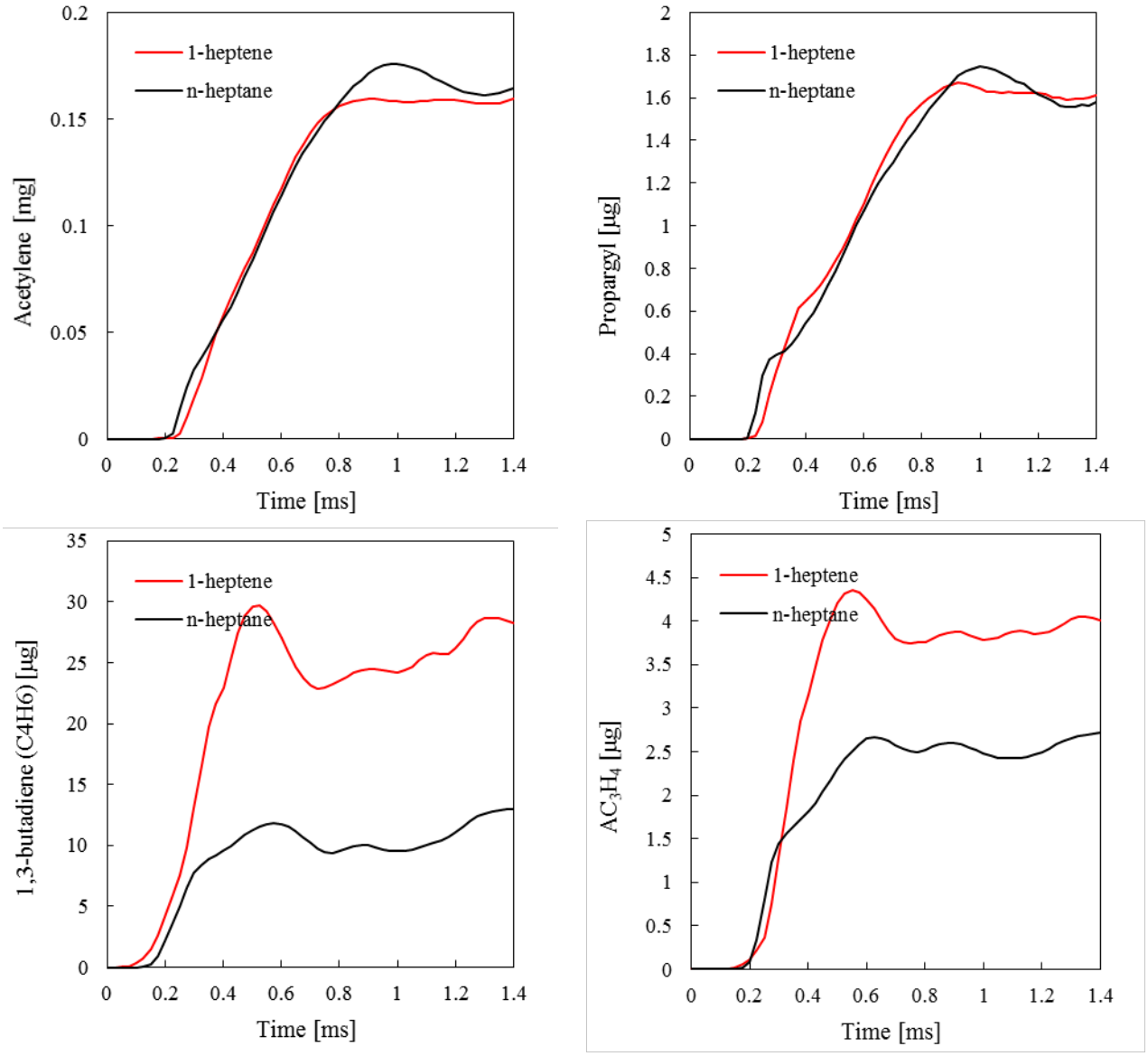


Fig. 18: Integrated mass of acetylene (C_2H_2), propargyl (C_3H_3), 1,3-butadiene (C_4H_6) and allene (AC_3H_4) in n-heptane and 1-heptane flames.