



Numerical study of soot formation in laminar coflow methane/air diffusion flames doped by *n*-heptane/toluene and iso-octane/toluene blends



Jean-Louis Consalvi^a, Fengshan Liu^{b,*}, M. Kashif^{c,d}, G. Legros^c

^aAix-Marseille Université, CNRS, IUSTI UMR 7343, 5 rue E. Fermi, 13013 Marseille, France

^bMeasurement Science and Standards, National Research Council of Canada, 1200 Montreal Road, Ottawa, Ontario K1A 0R6, Canada

^cSorbonne Universités, UPMC Univ Paris 06, CNRS, UMR 7190 Institut Jean le Rond d'Alembert, F-75005 Paris, France

^dMechanical Department, Faculty of Engineering, University of Central Punjab, 1 Khayaban-e-Jinnah, Johar Town, Lahore, Pakistan

ARTICLE INFO

Article history:

Received 12 July 2016

Revised 25 August 2016

Accepted 1 March 2017

Keywords:

Laminar coflow diffusion flame

Gasoline surrogate

Toluene reference fuels

PAH-based soot model

Synergistic effects

ABSTRACT

The laminar coflow nitrogen-diluted methane/air diffusion flames doped with a small amount of *n*-heptane/toluene and iso-octane/toluene binary mixtures, investigated experimentally by Kashif et al. (2015), were simulated numerically by using a detailed reaction mechanism and a sectional polycyclic aromatic hydrocarbon (PAH)-based soot model. The numerical model provides results in reasonable qualitative agreement with the experimental data by using the same chemical mechanism, the same soot model, and the same set of constants employed successfully in a previous study to model the effects of *n*-heptane/iso-octane doping, demonstrating that this overall model is promising to model soot formation in gasoline flames. Soot production is enhanced monotonically with increasing the toluene content in either the *n*-heptane/toluene or iso-octane/toluene doping fuel mixture. The increase in benzene and pyrene production displays a non-monotonic and synergistic response to the increase in toluene content. These numerical results are consistent with available experimental results as far as the trends in the effects of increasing the toluene content are concerned. Model results show that the dominant pathways responsible for the synergistic effects on benzene and pyrene production are respectively $C_6H_5CH_3$ (toluene) + H \leftrightarrow A1 (benzene) + CH₃ and A3- (C₁₄H₉) + C₂H₂ \leftrightarrow A4 (pyrene) + H.

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1. Introduction

Emissions of soot produced during incomplete combustion from various combustion systems, such as internal combustion engines and biomass burning, into the atmosphere have become a serious environment and health concern worldwide [1,2]. The transportation sector is largely responsible for black carbon emissions in developed countries and most of the on-road vehicles are powered by gasoline engines. The newly developed gasoline direct injection (GDI) engines offer better fuel economy by about 5 to 15% as compared to the traditional port fuel injection (PFI) gasoline engines, which helps lower CO₂ emissions. Unfortunately, GDI engines emit much more soot due to the stratified combustion mode in such engines. It is therefore desirable to understand the effects of various physical and chemical factors on soot formation to reduce soot emissions. Although it is important to investigate the effects of

these factors on soot emissions from GDI engines, it is challenging to isolate the influence of a particular factor, such as fuel chemistry, on soot formation, as the high sensitivity of soot emissions from a GDI engine to various engine parameters can mask the effect of this particular factor on soot formation. In order to circumvent this drawback, well-controlled laminar diffusion flames have been often used [3–7].

Gasoline consists of hundreds of aliphatic and aromatic hydrocarbon species. In order to make CFD analysis of gasoline engine performance and pollutants emissions tractable, it is necessary to develop surrogate fuel models, i.e., a simple mixture of few hydrocarbon compounds formulated in such a way that it has similar physical, chemical, and combustion characteristics as the real fuel. The primary constituents of gasoline are *n*-heptane (nC₇H₁₆), iso-octane (iC₈H₁₈) and toluene (C₆H₅CH₃) [8]. The binary mixtures of *n*-heptane and iso-octane are referred to as the primary reference fuels (PRF) for octane ratings. A binary mixture of *n*-heptane and iso-octane corresponds to a particular octane number or octane rating. Most gasoline surrogates are composed of toluene (C₆H₅CH₃), iso-octane (i-C₈H₁₈), and *n*-heptane

* Corresponding author. Fax: +16139577869.

E-mail address: fengshan.liu@nrc-cnrc.gc.ca (F. Liu).

(C₇H₁₆), also known as toluene reference fuels (TRFs) [8–12]. This has motivated the development of full and skeletal kinetic mechanisms for gasoline surrogates involving polycyclic aromatic hydrocarbons (PAHs), which are a prerequisite to model soot production [3,12–14].

Several experimental studies based on well-controlled laminar diffusion flames and aiming to understand soot formation in gasoline surrogates were reported. The sooting tendencies of gasoline, diesel, jet-A fuels and their surrogates were experimentally investigated in a laminar coflow heated methane/air diffusion flame at atmospheric pressure by doping methane with a small amount of vaporized liquid fuels (2200–2300 ppm) [4]. Kashif et al. conducted similar experiments to characterize the fuel sooting propensity of binary mixtures of *n*-heptane and iso-octane, *n*-heptane and toluene, and iso-octane and toluene [5,6]. They considered laminar CH₄/air coflow diffusion flames doped with these vaporized binary mixtures. The sooting tendency of these binary mixtures was determined by considering the Yield Sooting Indices (YSI) based on *n*-hexane and benzene. The soot production tendency of PRF was found to increase linearly with the volume fraction of iso-octane [5]. In contrast, the sooting tendency of *n*-heptane/toluene and iso-octane/toluene mixtures was found to increase in a non-linear and monotonic fashion with the toluene mole fraction [6]. In other words, the peak soot volume fraction in these binary mixture doped flames was found to be higher than that from a simple linear-by-volume model. In addition, the experimental data showed a larger degree of non-linear behaviour in iso-octane/toluene mixtures than that in *n*-heptane/toluene mixtures [6]. The non-linear variation of the peak soot volume fraction with toluene content in the binary mixtures is consistent with the experimental study of Choi et al. [3] conducted in *n*-heptane/toluene and iso-octane/toluene mixtures in soot formation/soot oxidation counterflow diffusion flames. Moreover, the experimental results of Choi et al. [3] showed that there exists a synergistic effect in PAH production in these mixtures, especially in iso-octane/toluene mixture, but not in soot formation. The synergistic effect is defined in a consistent manner with previous studies on soot and PAH formation and refers to the case when a mixture fuel (containing two hydrocarbons) can produce more PAH and/or soot as compared to the individual pure fuels [3,14–18]. This study intends to gain fundamental understanding into the effects of fuel chemistry of a TRF gasoline surrogate on soot formation. In particular, the focus is on the chemical kinetic interactions between iso-octane and toluene and between *n*-heptane and toluene with respect to PAH and soot formation. This study is complementary to the previous studies [5,19], where soot formation in laminar coflow methane/air diffusion flames doped with iso-octane and *n*-heptane blends was conducted experimentally and numerically, to gain a more comprehensive understanding of soot formation in diffusion flames fuelled with binary mixtures of TRF components.

2. Experiments

The laminar coflow diffusion flames studied experimentally by Kashif and coworkers [6] are simulated. In these experiments, measurements of soot volume fraction distribution were conducted in laminar coflow nitrogen-diluted methane diffusion flames doped with binary mixtures of either *n*-heptane and toluene or iso-octane and toluene at atmospheric pressure. The oxidizer is pure air. The composition of the binary mixture is identified by the volume fraction of toluene, X_{tol} , which is varied between 0 (pure *n*-heptane or iso-octane) and 1 (pure toluene). The burner consists of two concentric steel tubes of 11 mm (for fuel) and 102-mm (for oxidizer) inner diameter, respectively. The carrier gas, with a composition of 50% methane/50% nitrogen by volume, and the dopant (binary mixtures of *n*-heptane/toluene or iso-octane/toluene) flow through

the central fuel tube and their volumetric flow rates are kept at 400 cm³/min and 10.13 cm³/min (at 20 °C and 1 atm), respectively. This leads to a mole fraction of the vaporized binary fuel mixture of 2.47×10^{-2} in the fuel stream. The fuel line is maintained at about 423 K to prevent the condensation of the dopant.

The distribution of soot volume fraction was measured by a 2D light extinction measurement (LEM) technique at 645 nm. The value of the soot absorption refractive index function, $E(m)$, corrected to take into account the contribution of scattering ($1 + \alpha_{sa}E(m)$), where α_{sa} is the relative contribution of scattering to extinction) is taken equal to 0.28 for *n*-heptane and iso-octane and 0.308 for toluene [6]. For binary mixtures of *n*-heptane/toluene and iso-octane/toluene, this value is assumed to vary linearly with X_{tol} . It should be pointed out that varying the refraction index from 0.28 to 0.308 as X_{tol} varies from 0 to 1 modifies the measurements of soot volume fraction by only about 10 %, which is significantly less than the experimental uncertainty related to the value of $E(m)$ itself. Further details of the experimental setup and soot measurements using the LEM technique can be found in [5,6].

3. Numerical model

The governing equations and solution method have been given in previous studies [7,19,20] and will be described only briefly. The numerical model solves the conservation equations for mass, momentum, gas-phase species mass fraction, and energy in the low Mach number formulation and in axisymmetric coordinates by using a finite volume method and the SIMPLE algorithm. Additional transport equations for sectional soot aggregate and primary particle number densities are solved to describe the soot particle dynamics [7]. The divergence of the radiative flux was computed by the discrete ordinate method coupled to a statistical narrow-band-correlated k-based wide-band model for properties of CO, CO₂, and H₂O [21]. The spectral absorption coefficient of soot was obtained by Rayleigh's theory.

The reaction mechanism was assembled by merging the PAH formation and growth sub-mechanism developed at DLR [22,23] to the non-PAH part of a shortened version of the mechanism developed by Raj et al. [14] for gasoline surrogate fuel involving mixtures of *n*-heptane, iso-octane, and toluene. The shortened version of Raj et al. mechanism was described in [24] and the assembled hybrid mechanism for gasoline surrogate based on the DLR PAH sub-mechanism and the shortened Raj et al. non-PAH mechanism was described in detail in [19]. The final mechanism consists of 175 chemical species and 1175 reactions. The validation of this mechanism has been documented by Raj et al. [14]. The replacement of the original PAH sub-mechanism of Raj et al. [14] by that of DLR is not expected to alter its performance in flame modelling other than concentrations of PAHs, which are in general very low. As a validation study, the shortened Raj et al. mechanism described in [24] and the combined mechanism were used to predict the flame structure of a laminar premixed *n*-heptane flame and the predicted mole fraction distributions of several hydrocarbon species are compared with available experimental data in the Supplementary Information.

The fixed sectional soot model has been used and described in several previous studies, e.g. [20]. The range of soot aggregate mass is divided into a number of discrete sections, each with a prescribed representative mass [20]. In each section, all the soot aggregates are assumed to be identical and to be comprised of equally sized spherical primary particles and to have a fractal dimension of 1.8. The evolution of each section is governed by two transport equations for the number densities of soot aggregate and primary particle [20]. The incipient soot particles are assumed to be spherical and belong to the first section. As in previous studies [7,19–21], 35 sections were used with a spacing factor of 2.35.

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