

A Numerical Investigation on the Effect of Steam Injection Temperature in Soot Formation of a Steam-Assisted Lab-Scale Turbulent Diffusion Flame

Rahul Ramadas¹, Varunkumar S²

^{1,2}Thermodynamics and Combustion Engineering Lab
Indian Institute of Technology, Madras, Chennai, India
me22s035@smail.iitm.ac.in; varuns@smail.iitm.ac.in

Extended Abstract

Numerous experimental and numerical studies have been carried out to understand how water vapor influences the soot formation process in different fuel compositions and working conditions. The studies carried out by Frenklach and his team [1] provide a deeper insight into the soot formation via nucleation and surface growth, which is famously known as the HACA - Hydrogen Abstraction Acetylene Addition mechanism, which proposes a repetitive sequential process of hydrogen abstraction from an aromatic species to form an aromatic radical in the presence of an H radical, followed by the addition of a gaseous acetylene (C_2H_2) molecule at the radical site. The earlier studies concluded that water, both in liquid and gaseous forms, not only acted as a diluent but actively took part in the combustion reaction process. The injected H_2O reacts with the H and O free radicals in the combustion zone, resulting in the depletion of their concentration and an increase in the OH radical concentration, which also results in the reduction of C_2H_2 concentration. The reduction in C_2H_2 further lowered the propargyl (C_3H_3) concentration, thereby suppressing the benzene (C_6H_6) formation by their self-combination [2], [3].

The study presented here numerically investigates how the quantity and temperature of steam injected into the combustion zone influence the soot formation in a turbulent C_2H_4 /air diffusion flame. The study targets to understand how the soot formation phenomena in combustion systems respond to the temperature of the steam injected, the understanding of which can play an essential role in the reduction of soot from the combustion systems, especially the flaring systems employed vastly in the energy and industrial sectors, which contributes the majority of the soot and black carbon emissions.

The data from experiments carried out by Köhler et al. [4] and the numerical data from Blacha *et al.* [5] are utilized to assess the turbulence, chemistry, and soot models used in the present study. The computational domain is a 2-dimensional axisymmetric domain extending to 300D and 50D in axial and radial directions, where D is the diameter of the fuel jet from [4]. A two-equation k - ϵ model is used for modeling the turbulence field. The turbulence-chemistry interaction is modelled using the Steady Flamelet Model, and kinetics is represented using the detailed ABF mechanism [6]. A semi-empirical, two-equation Moss-Brookes model [7] is employed for modeling the soot formation process, which acknowledges the subprocesses involved in soot formation, such as nucleation, coagulation, surface growth, and oxidation.

The preliminary observations of the numerical results confirm that the steam injection has a significant effect in reducing the soot formation in the turbulent C_2H_4 /air diffusion flame. The soot volume fraction (svf) gives a clear indication of reduction in the maximum svf as we increase the quantity of steam injected. The numerical results also indicate that the steam temperature influences the soot formation in the turbulent C_2H_4 /air diffusion flame. Multiple numerical simulations have been performed by injecting an equal quantity of steam, by mass at various temperatures. The numerical simulation results indicate a decline in the peak svf as the temperature of the injected steam is increased. This implies that the increase in steam temperature has a suppressing effect on soot formation.

References

- [1] M. Frenklach, "Reaction mechanism of soot formation in flames," in *Physical Chemistry Chemical Physics*, 2002, pp. 2028–2037. doi: 10.1039/b110045a.
- [2] F. Liu, J. L. Consalvi, and A. Fuentes, "Effects of water vapor addition to the air stream on soot formation and flame properties in a laminar coflow ethylene/air diffusion flame," *Combust Flame*, vol. 161, no. 7, pp. 1724–1734, 2014, doi: 10.1016/j.combustflame.2013.12.017.
- [3] Y. Zhang, L. Wang, P. Liu, B. Guan, H. Ni, Z. Huang, H. Lin, "Experimental and kinetic study of the effects of CO₂ and H₂O addition on PAH formation in laminar premixed C₂H₄/O₂/Ar flames," *Combust Flame*, vol. 192, pp. 439–451, Jun. 2018, doi: 10.1016/j.combustflame.2018.01.050.
- [4] M. Köhler, K. P. Geigle, W. Meier, B. M. Crosland, K. A. Thomson, and G. J. Smallwood, "Sooting turbulent jet flame: Characterization and quantitative soot measurements," in *Applied Physics B: Lasers and Optics*, Aug. 2011, pp. 409–425. doi: 10.1007/s00340-011-4373-y.
- [5] T. Blacha, M. Di Domenico, M. Köhler, P. Gerlinger, and M. Aigner, "Soot Modeling in a Turbulent Unconfined C₂H₄/Air Jet Flame," 2011.
- [6] J. Jo, J. Appel, H. Bockhorn, and M. Frenklach, "Kinetic Modeling of Soot Formation with Detailed Chemistry and Physics: Laminar Premixed Flames of C₂ Hydrocarbons," 2000.
- [7] S. J. Brookes and J. B. Moss, "Predictions of Soot and Thermal Radiation Properties in Confined Turbulent Jet Diffusion Flames," 1999.