

INVESTIGATION OF THE EFFECT OF DIMETHYLETHER ADDITION ON THE KINETICS OF SOOT FORMATION IN A STANDARD PREMIXED ETHYLENE/AIR FLAT LAMINAR FLAME

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Abstract: The article presents the results of experimental study of soot formation with addition of dimethyl ether (from 0% to 100%) to the ethylene/air premixed flame. The volume fraction of the condensed phase was determined using the laser extinction method at a wavelength of 520 nm. The flame temperature profiles in the flame central axis were measured using thermocouples. It is shown that addition of dimethyl ether to ethylene flame leads to a change in the temperature profile in the flame and to a significant decrease in the volume fraction of condensed phase. With the substitution of 30% to 60% ethylene by dimethyl ether, a decrease in the volume fraction of soot to 0.01 ppm was observed, which is an order of magnitude less than this value in pure ethylene/air flame. Kinetic modeling of the growth of the volume fraction of soot in all investigated flames was carried out using the kinetic mechanisms CRECK and OpenSMOKE ++ software. Good agreement was obtained between the experimental and calculated data for ethylene/air flames and flames with additions of 15% to 60% dimethyl ether. For flames of 75% and 90% dimethylether + ethylene, and 100% dimethyl ether with air, experimental values of soot volume fraction were below the measurement sensitivity limit, and the calculated values indicated a decrease in the volume fraction by more than two orders of magnitude relative to a pure ethylene/air flame.

Keywords: premixed ethylene/dimethylether/air flame; volume fraction; soot; kinetic modeling

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Figure Captions

Figure 1 Profiles of the axial temperature (a) and of laser extinction at a wavelength of 520 nm (b) of the investigated flames depending on the height above a burner. Fuel compositions: 1 – 100% C₂H₄; 2 – 85% C₂H₄ + 15% DME; 3 – 70% C₂H₄ + 30% DME; 4 – 55% C₂H₄ + 45% DME; 5 – 40% C₂H₄ + 60% DME; 6 – 25% C₂H₄ + 75% DME; 7 – 10% C₂H₄ + 90% DME; and 8 – 100% DME

Figure 2 Volume fraction of condensed soot particles in the investigated flames depending on the height above a burner *H* (1 – experiment; and 2 – calculation): (a) 100% C₂H₄/air; (b) 85% C₂H₄ + 15% DME/air; (c) 70% C₂H₄ + 30% DME/air; (d) 55% C₂H₄ + 45% DME/air; (e) 40% C₂H₄ + 60% DME/air; (f) 25% C₂H₄ + 75% DME/air; (g) 10% C₂H₄ + 90% DME/air; and (h) 100% DME/air

Figure 3 The final maximum value of the volume fraction of soot at a height of 22 mm above a burner depending on the DME content: 1 – experimental measurements by laser light extinction; and 2 – calculation

Figure 4 The results of calculating the volume fraction of the condensed phase from the height above a burner in the DME/air flame using the temperature profiles shown in Fig. 1a: 1 – profile 1; and 2 – profile 8

Table Caption

Compositions of the investigated flames

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References

1. Inal, F., and S. M. Senkan. 2002. Effects of oxygenate additives on polycyclic aromatic hydrocarbons (PAHs) and soot formation. *Combust. Sci. Technol.* 174(9):1–19. doi: 10.1080/00102200290021353.
2. Sorenson, S. C. 2001. Dimethyl ether in diesel engines: Progress and perspectives. *Transactions ASME* 123:652–658. doi: 10.1115/1.1370373.

3. Wu, J., K. H. Song, T. Litzinger, S.-Y. Lee, R. Santoro, and M. Linevsky. 2006. Reduction of PAH and soot in premixed ethylene–air flames by addition of dimethyl ether. *Combust. Sci. Technol.* 178:837–863. doi: 10.1080/00102200500269942.
4. McEnally, C. S., and L. D. Pfefferle. 2007. The effects of dimethyl ether and ethanol on benzene and soot formation in ethylene nonpremixed flames. *P. Combust. Inst.* 31(1):603–610. doi: 10.1016/j.proci.2006.07.005.
5. Liu, F., X. He, X. Ma, Q. Zhang, M. J. Thomson, H. Guo, G. J. Smallwood, S. Shuai, and J. Wang. 2011. An experimental and numerical study of the effects of dimethyl ether addition to fuel on polycyclic aromatic hydrocarbon and soot formation in laminar coflow ethylene/air diffusion flames. *Combust. Flame* 158(3):547–563. doi: 10.1016/j.proci.2006.07.005.
6. Sirignano, M., M. Salamanca, and A. D’Anna. 2014. The role of dimethyl ether as substituent to ethylene on particulate formation in premixed and counter-flow diffusion flames. *Fuel* 126:256–262. doi: 10.1016/j.fuel.2014.02.039.
7. Choi, J. H., B. C. Choi, S. M. Lee, S. H. Chung, K. S. Jung, W. L. Jeong, S. K. Choi, and S. K. Park. 2015. Effects of DME mixing on number density and size properties of soot particles in counterflow non-premixed ethylene flames. *J. Mech. Sci. Technol.* 29(5):2259–2267. doi: 10.1007/s12206-015-0447-9.
8. Kang, Y., Y. Sun, X. Lu, X. Gou, S. Sun, J. Yan, Y. Song, P. Zhang, Q. Wang, and X. Ji. 2018. Soot formation characteristics of ethylene premixed burner-stabilized stagnation flame with dimethyl ether addition. *Energy* 150:709–721. doi: 10.1016/j.energy.2018.03.025.
9. Zhang, Y., Y. Li, P. Liu, R. Zhan, Z. Huang, and H. Lin. 2019. Investigation on the chemical effects of dimethyl ether and ethanol additions on PAH formation in laminar premixed ethylene flames. *Fuel* 256:115809. doi: 10.1016/j.fuel.2019.115809.
10. Li, Z., P. Liu, P. Zhang, Y. Wang, H. He, S. H. Chung, and W. L. Roberts. 2020. Role of dimethyl ether in incipient soot formation in premixed ethylene flames. *Combust. Flame* 216:271–279. doi: 10.1016/j.combustflame.2020.03.004.
11. Ahmed, H. A., M. A. Ashraf, S. A. Steinmetz, M. J. Dunn, and A. R. Masri. 2021. The role of DME addition on the evolution of soot and soot precursors in laminar ethylene jet flames. *P. Combust. Inst.* 38(4):5319–5329. doi: 10.1016/j.proci.2020.06.055.
12. ISF-2019. University of Adelaide. Available at: <https://www.adelaide.edu.au/cet/isfworkshop/data-sets/laminar-flames#isf-4-premixed-flames-3-mckenna-burner-stabilised-flames-lii-target-flames> (accessed November 15, 2021).
13. McEnally C. S., Köylü Ü.Ö., Pfefferle L. D., and Rosner D. E. 1997. Soot volume fraction and temperature measurements in laminar nonpremixed flames using thermocouples. *Combust. Flame* 109:701–720. doi: 10.1016/S0010-2180(97)00054-0.
14. Eremin, A. V., E. V. Gurentsov, and R. N. Kolotushkin. 2020. The change of soot refractive index function along the height of premixed ethylene/air flame and its correlation with soot structure. *Appl. Phys. B* 126:125. doi: 10.1007/s00340-020-07426-3.
15. Cuoci, A., A. Frassoldati, T. Faravelli, and E. Ranzi. 2015. OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms. *Comput. Phys. Commun.* 192:237–264. doi: 10.1016/J.CPC.2015.02.014.
16. Smooke, M., I. Puri, and K. Seshadri. 1986. A comparison between numerical calculations and experimental measurements of the structure of a counterflow diffusion flame burning diluted methane in diluted air. *P. Combust. Inst.* 21:1783–1792. doi: 10.1016/S0082-0784(88)80412-0.
17. Abid, A. D., J. Camacho, D. A. Sheen, and H. Wang. 2009. Quantitative measurement of soot particle size distribution in premixed flames — the burner-stabilized stagnation flame approach. *Combust. Flame* 156:1862–1870. doi: 10.1016/j.combustflame.2009.05.010.
18. Burke, U., K. P. Somers, P. O’Toole, C. M. Zinner, N. Marquet, G. Bourque, E. L. Petersen, W. K. Metcalfe, Z. Serinyel, and H. J. Curran. 2015. An ignition delay and kinetic modeling study of methane, dimethyl ether, and their mixtures at high pressures. *Combust. Flame* 162(2):315–330. doi: 10.1016/j.combustflame.2014.08.014.
19. Pejpichestakul, W., E. Ranzi, M. Pelucchi, A. Frassoldati, A. Cuoci, A. Parente, and T. Faravelli. 2019. Examination of a soot model in premixed laminar flames at fuel-rich conditions. *P. Combust. Inst.* 37(1):1013–1021. doi: 10.1016/j.proci.2018.06.104.
20. Ranzi, E., A. Frassoldati, R. Grana, A. Cuoci, T. Faravelli, A. P. Kelley, and C. K. Law. 2012. Hierarchical and comparative kinetic modeling of laminar flame speeds of hydrocarbon and oxygenated fuels. *Prog. Energ. Combust.* 38:468–501. doi: 10.1016/j.pecs.2012.03.004.
21. Saggese, C., A. Frassoldati, A. Cuoci, T. Faravelli, and E. Ranzi. 2013. A wide range kinetic modeling study of pyrolysis and oxidation of benzene. *Combust. Flame* 160:1168–1190. doi: 10.1016/j.combustflame.2013.02.013.
22. Saggese, C., N. E. Sanchez, A. Frassoldati, A. Cuoci, T. Faravelli, M. U. Alzueta, and E. Ranzi. 2014. Kinetic modeling study of polycyclic aromatic hydrocarbons and soot formation in acetylene pyrolysis. *Energ. Fuel.* 28:1489–1501. doi: 10.1021/ef402048q.
23. Kee, R. J., F. M. Rupley, and J. A. Miller. 1989. CHEMKIN-II: A FORTRAN Chemical Kinetics Package for the Analysis of Gas-Phase Chemical Kinetics. Albuquerque, NM. Sandia Report No. 89-8009B.
24. Burcat, A., and B. Ruscic. 2005. Third millennium ideal gas and condensed phase thermochemical database for combustion with updates from active thermochemical tables. Argonne, IL: Argonne National Laboratory. doi: 10.2172/925269.

25. Saggese, C., S. Ferrario, J. Camacho, A. Cuoci, A. Frassoldati, E. Ranzi, H. Wang, and T. Faravelli. 2015. Kinetic modeling of particle size distribution of soot in a premixed burner-stabilized stagnation ethylene flame. *Combust. Flame* 162:3356–3369. doi: 10.1016/j.combustflame.2015.06.002.

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