

SPHERICAL DIFFUSION FLAMES: SOOT FORMATION

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Abstract: The joint American–Russian space experiment (SE) Flame Design (Adamant) was carried out on the International Space Station (ISS) in the period from 2019 to 2022. The objective of the joint SE was to study the mechanisms of control of soot formation in a spherical diffusion flame (SDF) formed around a porous sphere (PS) and radiative extinction of the SDF under microgravity conditions. The objects of the study were “normal” and “inverse” SDFs of gaseous ethylene in an oxygen atmosphere with nitrogen addition at room temperature and pressures ranging from 0.5 to 2 atm. A normal flame is a flame formed in an oxidizing atmosphere when fuel is supplied through the PS. An inverse flame is a flame formed in a fuel atmosphere when an oxidizer is introduced through the PS. Presented in the paper are the results of calculations of soot formation in normal and inverse SDFs. The calculations are based on a one-dimensional nonstationary model of diffusion combustion of gases with detailed kinetics of ethylene oxidation supplemented with a macrokinetic mechanism of soot formation. It is shown that soot formation in normal and inverse SDFs is concentrated in the region where the local C/O atomic ratio and local temperature satisfy the conditions $0.32 < \text{C}/\text{O} < 0.44$ and $T > 1300–1500$ K.

Keywords: space experiment; microgravity; spherical diffusion flame; ethylene; numerical simulation; soot formation; radiative flame extinction

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Figure Captions

Figure 1 Photograph of the PS mounted on a gas supply tube (*a*) and the schematic of the computational domain (*b*)

Figure 2 Photographs of the SDFs of ethylene in the Flame Design (Adamant) SE under microgravity conditions on the ISS: (*a*) sooty normal flame; and (*b*) sooty inverse flame [26, 27]

Figure 3 Examples of the time histories of the flame radius: (*a*) normal flame (19142J3); (*b*) inverse flame (22018G2); signs — experiment; and curves — calculation

Figure 4 Examples of the time histories of the flame temperature: (*a*) normal flame (19142J3); (*b*) inverse flame (22018G2); signs — experiment; and curves — calculation

Figure 5 Examples of time histories of the size (*a*) and temperature (*b*) of a quasi-stationary inverse flame (21328D1): signs — experiment; and curves — calculation

Figure 6 Calculated time histories of the temperature of normal (*1*) and inverse (*2*) flames undergoing radiative extinction

Figure 7 Typical calculated structures of normal (19171D4) (*a*) and inverse (22018G2) (*b*) diffusion flames in 20 s after ignition: *1* — $Y_{\text{C}_2\text{H}_4}$; *2* — Y_{O_2} ; *3* — Y_{N_2} ; *4* — Y_{CO_2} ; *5* — $Y_{\text{H}_2\text{O}}$; *6* — Y_{CO} ; *7* — Y_{OH} ; and *8* — $Y_{\text{soot}} \cdot 10^4$ (*a*) and $Y_{\text{soot}} \cdot 10^6$ (*b*)

Figure 8 Dynamics of change in the calculated total soot mass $m_{\text{soot},\Sigma}$ vs. time for normal (*1*) and inverse (*2*) flames with different values of Z_{st} : (*a*) $t = 1$ s; (*b*) 5; (*c*) 10; (*d*) 15; (*e*) 20; (*f*) 25; (*g*) 30; (*h*) 35; (*i*) 40; (*j*) 45; (*k*) 50; (*l*) $t = 1$ s

Figure 9 The normalized cumulative rate of soot formation $\dot{m}_{\text{soot},\Sigma}(t)$ in normal (*1*) and inverse (*2*) flames listed in Tables 2 and 3 as a function of the instantaneous local gas temperature at the point of maximum soot mass fraction in the flame structure

Figure 10 Calculated dependences of the cumulative rate of soot formation $\dot{m}_{\text{soot},\Sigma}(t)$ on the C/O atomic ratio and temperature at the point of maximum soot concentration in the flame structure at different times after ignition: (*a*) 2 s; (*b*) 5; (*c*) 10 s; *1* — $\dot{m}_{\text{soot},\Sigma}(t) > 0$; *2* — $\dot{m}_{\text{soot},\Sigma}(t) < 0$

Figure 11 Calculated dependences of temperature on the local C/O atomic ratio (*a*) and temperature $T_{0.53}$ and atomic ratio $(\text{C}/\text{O})_{1305}$ on the stoichiometric mixture fraction Z_{st} (*b*) in normal (*1*) and inverse (*2*) flames in 2 s after ignition [20]

Figure 12 Calculated dependences of temperature on the local C/O atomic ratio in normal (black curves) and inverse (grey curves) flames in 2 (*a*), 10 (*b*), 20 (*c*), and 30 s (*d*) after ignition. The regions colored with semitransparent grey fill correspond to the parametric domains of soot formation

Table Captions

Table 1 Macrokinetic mechanism of soot formation

Table 2 Conditions for normal flames

Table 3 Conditions for inverse flames

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References

1. Haynes, B. S., and H. Gh. Wagner. 1981. Soot formation. *Prog. Energ. Combust.* 7:229–273.
2. Kennedy, I. M. 1997. Models of soot formation and oxidation. *Prog. Energ. Combust.* 23:95–132.
3. Richter, H., and J. B. Howard. 2000. Formation of polycyclic aromatic hydrocarbons and their growth to soot – a review of chemical reaction pathways. *Prog. Energ. Combust.* 26:565–608. doi: 10.1016/S0360-1285(00)00009-5.
4. Karatas, A. E., and Ö. L. Gülder. 2012. Soot formation in high pressure laminar diffusion flames. *Prog. Energ. Combust.* 38:818–845. doi: 10.1016/j.pecs.2012.04.003.
5. Wang, Y., and S. H. Chung. 2019. Soot formation in laminar counterflow flames. *Prog. Energ. Combust.* 74:152–238. doi: 10.1016/j.pecs.2019.05.003.
6. Lapuerta, M., J. Rodríguez-Fernández, J. Sánchez-Valdepeñas. 2020. Soot reactivity analysis and implications on diesel filter regeneration. *Prog. Energ. Combust.* 78:100833. doi: 10.1016/j.pecs.2020.100833.
7. Martin, J. W., M. Salamanca, and M. Kraft. 2022. Soot inception: Carbonaceous nanoparticle formation in flames. *Prog. Energ. Combust.* 88:100956. doi: 10.1016/j.pecs.2021.100956.
8. Santoro, R. J., T. T. Yeh, J. J. Horvath, and H. G. Seumerjian. 1987. The transport and growth of soot particles in laminar diffusion flames. *Combust. Sci. Technol.* 53(2-3):89–115. doi: 10.1080/00102208708947022.
9. Glassman, I. 1989. Soot formation in combustion processes. *P. Combust. Inst.* 22(1):295–311. doi: 10.1016/S0082-0784(89)80036-0.
10. Glassman, I., O. Nishida, and G. Sidebotham. 1994. Critical temperatures of soot formation. *Soot formation in combustion*. Ed. H. Bockhorn. Springer ser in chemical physics. Springer. 59:316–324. doi: 10.1007/978-3-642-85167-4_18.
11. Sunderland, P. B., and G. M. Faeth. 1996. Soot formation in hydrocarbon/air laminar jet diffusion flames. *Combust. Flame* 105(1-2):132–146. doi: 10.1016/0010-2180(95)00182-4.
12. Glassman, I. 1998. Sooting laminar diffusion flames: Effect of dilution, additives, pressure, and microgravity. *27th Symposium (International) on Combustion Proceedings.* 27(1):1589–1596. doi: 10.1016/s0082-0784(98)80568-7.
13. Atreya, A., S. Agrawal, K. Sacksteder, and H. Baum. 1994. Observations of methane and ethylene diffusion flames stabilized around a blowing porous sphere under microgravity conditions. AIAA Paper No. 94-0572.
14. Tse, S. D., D. Zhu, C.-J. Sung, Y. Ju, and C. K. Law. 2001. Microgravity burner-generated spherical diffusion flames: Experiment and computation. *Combust. Flame* 125(4):1265–1278.
15. Sunderland, P. B., R. L. Axelbaum, D. L. Urban, B. H. Chao, and S. Liu. 2003. Effects of structure and hydrodynamics on the sooting behavior of spherical microgravity diffusion flames. *Combust. Flame* 132:25–33.
16. Santa, K. J., B. H. Chao, P. B. Sunderland, D. L. Urban, D. P. Stocker, and R. L. Axelbaum. 2007. Radiative extinction of gaseous spherical diffusion flames in microgravity. *Combust. Flame* 151(4):665–675.
17. Chernovsky, M. K., A. Atreya, and H. G. Im. 2007. Effect of CO₂ diluent on fuel versus oxidizer side of spherical diffusion flames in microgravity. *P. Combust. Inst.* 31(1):1005–1013.
18. Christiansen, E. W., S. D. Tse, and C. K. Law. 2003. A computational study of oscillatory extinction of spherical diffusion flames. *Combust. Flame* 134:327–337.
19. Liu, S., B. H. Chao, and R. L. Axelbaum. 2005. A theoretical study on soot inception in spherical burner-stabilized diffusion flames. *Combust. Flame* 140:1–23.
20. Lecoustre, V. R., P. B. Sunderland, B. H. Chao, and R. L. Axelbaum. 2012. Numerical investigation of spherical diffusion flames at their sooting limits. *Combust. Flame* 159:194–199.
21. Irace, P. H., H. J. Lee, K. Waddell, L. Tan, D. P. Stocker, P. B. Sunderland, and R. L. Axelbaum. 2021. Observations of long duration microgravity spherical diffusion flames aboard the International Space Station. *Combust. Flame* 229:111373.
22. Frolov, S. M., S. N. Medvedev, and F. S. Frolov. 2021. Sfericheskoe diffuzionnoe plamya etilena v kosmicheskikh eksperimentakh "Adamant" [Spherical diffusion flame of ethylene in the spaceflight experiment "Adamant"]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 14(1):9–21 doi: 10.30826/CE21140102.
23. Basevich, V. Ya., A. A. Belyaev, V. S. Posvyanskii, and S. M. Frolov. 2013. Mechanisms of the oxidation and combustion of normal paraffin hydrocarbons: transition from C₁–C₁₀ to C₁₁–C₁₆. *Russ. J. Phys. Chem. B* 7(2):161–169. doi: 10.1134/S1990793113020103.
24. Basevich, V. Ya., S. N. Medvedev, S. M. Frolov, F. S. Frolov, B. Basara, and P. Prieching. 2016. Makrokineticheskaya model' dlya rascheta emissii sazhi v dizele [Macrokinetic model for calculating soot emission in Diesel engine]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 9(3):36–46.

25. Agafonov, G. L., I. V. Bilera, P. A. Vlasov, Yu. A. Kolbanovskii, V. N. Smirnov, and A. M. Tereza. 2015. Soot formation during the pyrolysis and oxidation of acetylene and ethylene in shock waves. *Kinet. Catal.* 56(1): 12–30.
26. Space Flames. Available at: www.flickr.com/photos/space-flames (accessed November 20, 2022).
27. www.facebook.com/space.flames.
28. Minutolo, P., G. Gambi, and A. D'Alessio. 1998. Properties of carbonaceous nanoparticles in flat premixed C₂H₄/air flames with C/O ranging from 0.4 to soot appearance limit. *Symposium (International) on Combustion Proceedings* 27(1):1461–1469. doi: 10.1016/s0082-0784(98)80553-5.

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