TO THE STEADY STATE THEORY OF GAS IGNITION WITH A HEATED BODY

A. A. Belyaev and B. S. Ermolaev

N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

Abstract: Steady-state theory of ignition by a heated flat surface formulated by Ya. B. Zeldovich in 1939 played a pioneering role in the successful development of ignition of various combustible materials. The analytical solution obtained later for a cylindrical surface opened the opportunity of comparison with experimental data. In the work performed by Filippov et al., a discrepancy was found between experiments on the ignition of methane-air mixtures with heated wires and an analytical solution. Based on it, Filippov et al. expressed doubts about the correctness of the model. However, this discrepancy may be due to the fact that the experiment used for comparison with the model does not fully satisfy the limitations that follow from the simplifying assumptions made when formulating the model. These assumptions and the limitations that follow from them are analyzed in this paper in relation to Kumagai's experiments on the ignition of a methane-air mixture. Key assumptions of the steady-state model: a simplified description of the kinetics of chemical heat release using a global one-stage Arrhenius-type reaction without burnup; the condition that the thickness of the reaction zone must be substantially less than the thickness of the dynamic boundary layer; and the cylindrical symmetry of the thermal field around the heated body. Based on the analyses of the heat release kinetics, a numerical solution for two nonsteady problems of gas ignition with a heated body and gas self-ignition in a plug flow reactor with detailed reaction kinetics has been obtained. The solutions showed that the dependence of the heat release rate on temperature constructed for specific calculation options has a complex shape that cannot be even approximately described using the heat release law in the Arrhenius form. Nevertheless, it turned out that the critical Nusselt numbers delimiting the ignition region and the region of steady-state temperature profiles, which were calculated using the formulas of the analytical model with the appropriate procedure for calibrating the heat release characteristics, are in good agreement with the experimental data in the entire range of diameters and wire heating temperatures and gas flow rates. Also, good agreement with the experiment and the analytical model for critical ignition conditions was obtained in calculations using the unsteady ignition model, despite noticeable differences in the heat release rate depending on temperature. The condition of a small thickness of the reaction zone in relation to the size of the boundary layer is generally satisfied quite well, although at high gas flow velocities (at the level of 10 m/s), the mathematical rigor of this condition becomes insufficient for avoiding the convective heat transfer at the reaction zone. Due to separation of the flow from the body surface and formation of eddies, a region of reduced heat transfer is formed at the body surface near the azimuth angle of 90° . The value of this reduced heat transfer can be noticeably less than the average one. It is in these areas of the surface of a heated body that conditions favorable for ignition are created. If a correction is made with a corresponding reduction in the critical Nusselt numbers in these experiments, then this would weaken the dependence of the critical Nusselt number on the wire diameter observed in the experiment bringing it closer to the approximately proportional dependence that follows from the analytical solution.

Keywords: cylindrical heated surface; gas mixture; ignition criterion; analytical estimates; computer modeling; comparison with experiment

DOI: 10.30826/CE22150301

EDN: GAIHZT

Figure Captions

Figure 1 Photograph of the ignition of a gas mixture by the cylindrical hot wire in the experiment [3]

Figure 2 Examples of temperature (a) and temperature gradient (b) distributions along the radial coordinate calculated at $\xi_s = 3.2$, Nu = 1.6, and $\theta_0 = -13.7$: *I* and *2* are obtained with the signs "+" and "-" in Eq. (7), respectively; and θ - at C = 0 (critical ignition condition)

Figure 3 An example of the calculated distribution of temperature (1) and heat release rate (2) along the reactor axis for the self-ignition process in a plug flow reactor. The temperature and velocity of the gas at the inlet are 1324 K and 30 cm/s, respectively

GORENIE I VZRYV (MOSKVA) – COMBUSTION AND EXPLOSION 2022 volume 15 number 3

Figure 4 Temperature dependence of the ignition delay time; the delay time is determined by the temperature increase by 80% (1) and by the increase by 5 K (2). In both cases, E = 46.6 kcal/mol

Figure 5 Logarithmic dependence of the heat release rate on the reciprocal temperature for the self-ignition process in a plug flow reactor. The temperature and velocity of the gas at the inlet are 1324 K and 30 cm/s, respectively. Dashed line corresponds to the activation energy E = 74.8 kcal/mol

Figure 6 Comparison of temperature profiles for the variant with $T_s = 1405$ K, $d_s = 0.1$ cm, $r_0 = 0.35$ cm, and Nu = 1.2: calculations according to the numerical model when there is no ignition (1), according to the analytical steady state model (2), and according to Eq. (4) with boundary conditions (2)–(3) (3)

Figure 7 Calculation with numerical model at $d_s = 1$ mm, $T_s = 1537$ K, v = 10 m/s, and Nu = 4.3 without ignition. Distribution of heat release rate at 15 (1), 25 (2), and 30 ms (3)

Figure 8 Temperature dependence of the heat release rate: 1 - calculation with detailed kinetics for a flow reactor, initial temperature 1324 K, gas flow velocity 0.3 m/s; 2 - calculation with detailed kinetics in the *r* coordinate corresponding to the maximum temperature for gas ignition with a wire 1 mm in diameter and a temperature of 1324 K, the Nusselt number is below the critical value; 3 - dependence used in the analytical model, activation energy 46.6 kcal/mol; dotted line is drawn through the points of the calculated curve which correspond to an activation energy of 74.8 kcal/mol

Figure 9 Dependence of the critical Nusselt number on the wire diameter at different temperatures of the heated body: 1 - 1500 K; 2 - 1400; and 3 - 1350 K; solid lines – calculation according to the stationary ignition model; and dashed lines – experiment [3]

Figure 10 Experimental values of local Nusselt numbers in the flow around a circular cylinder at Reynolds numbers from 20 to 600 (from book [7])

Table Captions

 Table 1 Conditions and main characteristics of experiments

Table 2 Critical ignition conditions obtained in the experiment and in calculations using the numerical model and the analytical stationary model

Acknowledgments

The work was carried out within the framework of the Program of Fundamental Research of the Russian Federation (state registration numbers 122040500073-4 and 122040500068-0).

References

- 1. Zel'dovich, Ya. B. 1939. Teoriya zazhiganiya nakalennoy poverkhnost'yu [The theory of ignition by an incandescent surface]. *ZhETF* 9(12):1530–1534.
- 2. Zel'dovich, Ya. B., G. I. Barenblatt, V. B. Librovich, and G. M. Makhviladze. 1980. *Matematicheskaya teoriya goreniya i vzryva* [Mathematical theory of combustion and explosion]. Moscow: Nauka. 478 p.
- 3. Kumagai, S. 1979. *Gorenie* [Combustion]. Moscow: Khimiya. 256 p.
- 4. Philippov, A. A., and N. A. Khalturinskiy. 2015. To the theory of ignition by a hot surface: Critical conditions for occurrence of explosive and avalanche-like processes. *Zel'dovich Memorial: Accomplishments in the combustion science in the last decade*. Eds. A. A. Borisov and S. M. Frolov. Moscow: TORUS PRESS. 2:89–94.
- Philippov, A. A., and Al. Al. Berlin. 2021. K teorii zazhiganiya nakalennoy poverkhnost'yu [To the theory of ignition by hot surface]. *Goren. Vzryv (Mosk.) – Combustion and Explosion* 14(2):3–7.

- 6. Zel'dovich, Ya. B. 1984. *Izbrannye trudy. Khimicheskaya fizika i gidrodinamika* [Selected works. Chemical physics and hydrodynamics]. Moscow: Nauka. 374 p. (Kommentariy k stat'e "Teoriya zazhiganiya nakalennoy poverkhnost'yu" [Comment on the article "The theory of ignition by an incandescent surface"]. P. 225.)
- Gröber, H., S. Erk, and U. Grigull. 1955. *Die Grundgesetze der Wärmeübertragung.* – Berlin–Göttingen– Heidelberg: Springer. 428 p.
- 8. Frank-Kamenetskii, D. A. 1969. *Diffusion and heat transfer in chemical kinetics*. New York: NY: Plenum Press. 600 p.
- 9. ANSYS Academic Research CFD. CHEMKIN-Pro 15112, Reaction Design: San Diego, CK-TUT-10112-1112-UG-1, 2011.
- 10. Kutateladze, S. S. 1990. *Teploperedacha i gidrodinamicheskoe soprotivlenie* [Heat transfer and hydrodynamic resistance]. Moscow: Energoatomizdat. 367 p.
- 11. Reid, R. J., J. Prausnitz, and T. Sherwood. 1977. *Properties of gases & liquids*. New York, NY: McGraw Hill. 703 p.
- 12. Burcat, A. Ideal gas thermodynamic data in polynomial form for combustion and air pollution use. Available at:

http://garfield.chem.elte.hu/Burcat/burcat.html/ (accessed January 21, 2022).

- Tereza, A. M., G. L. Agafonov, A. S. Betev, and S. P. Medvedev. 2020. Reduction of the detailed kinetic mechanism for efficient simulation of ignition delay for mixtures of methane and acetylene with oxygen. *Russ. J. Phys. Chem. B* 14(6):951–958.
- Mechanism Downloads. 2018. AramcoMech 3.0 Available at: http://c3.nuigalway.ie/combustionchemistrycentre/ mechanismdownloads/ (accessed January 13, 2022).
- Arutyunov, V. S. 2011. Okislitel'naya konversiya prirodnogo gaza [Oxidative conversion of natural gas]. Moscow: KRASAND. 640 p.
- 16. Schlichting, G. 1979. *Boundary layer-theory*. McGraw-Hill, Inc. 817 p.

- 17. 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 C_1-C_{10} to $C_{11}-C_{16}$. *Russ. J. Phys. Chem. B* 7(2):161–169.
- Basevich, V. Ya., and S. M. Frolov. 2007. Kinetics of "blue" flames in the gas-phase oxidation and combustion of hydrocarbons and their derivatives. *Russ. Chem. Rev.* 76(9):867–884.
- Salgansky, E.A., M.V. Tsvetkov, A.Yu. Zaichenko, D.N. Podlesny, and I.V. Sedov. 2021. Thermodynamic evaluation of noncatalytic conversion of natural gas with the production of synthesis gas. *Russ. J. Phys. Chem. B* 15(6):969–976.

Received June 22, 2022

Contributors

Belyaev Andrey A. (b. 1954) — Candidate of Science in physics and mathematics, leading research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow, 119991, Russian Federation; belyaevIHF@yandex.ru

Ermolaev Boris S. (b. 1940) — Doctor of Science in physics and mathematics, leading research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow, 119991, Russian Federation; boris.ermolaev44@mail.ru