CONVERSION OF RICH PREHEATED METHANE–OXYGEN MIXTURES IN A FLAT STABILIZED LAMINAR FLAME

M. G. Bryukov[1], A. A. Belyaev[1], K. Ya. Troshin[1], P. A. Vlasov[1], and V. S. Arutyunov[1,2]

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

[2]Federal Research Center for Problems of Chemical Physics and Medicinal Chemistry of the Russian Academy of Sciences, 1 Prosp. Academician Semenov, Chernogolovka, Moscow Region 142432, Russian Federation

Abstract: The article presents the results of kinetic modeling of the process of conversion of rich preheated methane–oxygen mixtures into syngas in the flat stabilized laminar flame in the range of initial temperatures of 300–800 K, fuel-to-air equivalence ratio of 2.4–3.2, and at pressure of 1,5 atm. At the initial temperature of 800 K, the optimal value of the fuel-to-air equivalence ratio $\varphi = 2.77$ (air-to-fuel equivalence ratio $\alpha = 0.361$) is determined, at which the maximum conversion of methane into hydrogen of 79,9% is achieved and the conversion into carbon monoxide is close to the maximum and equals 93,5%. Moreover, with an almost complete conversion of methane of 99,3%, its conversion into carbon dioxide CO_2 is only 5,0% and into water — 19,6%. These results virtually coincide with the experimental results of matrix conversion of methane–oxygen mixtures into syngas, in which similar preliminary heating of the gas mixture to approximately the same temperature occurs due to internal heat recovery of hot syngas. The obtained results indicate the adequacy of the presented kinetic modeling of the processes of gas-phase oxidative conversion of methane into syngas.

Keywords: methane; oxygen; hydrogen; syngas; oxidation conversion; kinetic modeling

DOI: 10.30826/CE25180102 **EDN:** XPXJSO

Figure Captions

Figure 1 Profiles of temperature (*a*), velocity of the reacting mixture (*b*), and concentrations of reagents (*c*) and main products (*d*) of a stabilized flat laminar flame of a methane–oxygen mixture. Fuel-to-air equivalence ratio is 2.77, pressure is 1,5 atm, and initial temperature is 800 K. Signs — calculation results; curves — corresponding splines; and x — coordinate directed along the gas flow: $x = 0$ — burner inlet and $x = 10$ cm — burner outlet

Figure 2 Dependences of conversions of methane to hydrogen on the fuel-to-air equivalence ratio at pressure of 1.5 atm and initial gas temperatures of 300 (*1*), 600 (*2*), 700 (*3*), and 800 K (*4*): signs — calculation results; and curves — corresponding splines

Figure 3 Dependences of total methane conversion (*1*) and of conversions of methane into hydrogen (*2*), water (*3*), CO (*4*), and CO_2 (*5*) on the fuel-to-air equivalence ratio at pressure of 1.5 atm and initial gas temperature of 800 K: signs — calculation results; and curves — corresponding splines

Table Captions

Table 1 Initial flow rates of unburned gas which are set at the burner inlet

Table 2 Key reactions controlling the process of conversion of rich methane–oxygen mixtures at pressure of 1.5 atm and initial temperature of 800 K in the vicinity of the maximum of the derivative of the mole fraction of the hydroxyl radical with respect to the coordinate x

References

1. Aasberg-Petersen, K., I. Dybkjær, C. V. Ovesen, N. C. Schjødt, J. Sehested, and S. G. Thomsen. 2011. Natural gas to synthesis gas — catalysts and catalytic processes. *J. Nat. Gas Sci. Eng.* 3:423–459. doi: 10.1016/j.jngse.2011.03.004.
2. Dybkjær, I., and K. Aasberg-Petersen. 2016. Synthesis gas technology large-scale applications. *Can. J. Chem. Eng.* 94:607–612. doi: 10.1002/cjce.22453.
3. Arutyunov, V. S., I. A. Golubeva, O. L. Eliseev, and F. G. Zhagfarov. 2020. *Tekhnologiya pererabotki uglevodorodnykh gazov* [Technology of processing of hydrocarbon gases]. Moscow: Yurayt Publs. 723 p.
4. Arutyunov, V. S., V. M. Shmelev, I. N. Lobanov, and G. G. Politenkova. 2010. A generator of synthesis gas and hydrogen based on a radiation burner. *Theor. Found. Chem. Eng.* 44:20–29.
5. Arutyunov, V. S., V. M. Shmelev, M. Yu. Sinev, and O. V. Shapovalova. 2011. Syngas and hydrogen produc-

tion in a volumetric radiation burners. *Chem. Eng. J.* 176-177:291–294. doi: 10.1016/j.cej.2011.03.084.
6. Arutyunov, V. S., V. I. Savchenko, I. V. Sedov, V. M. Shmelev, A. V. Nikitin, I. G. Fokin, S. A. Eksanov, O. V. Shapovalova, and K. A. Timofeev. 2016. Experimental studies of natural gas to synthesis gas converters based on permeable cavity matrixes. *Russ. J. Appl. Chem.* 89:1816–1824. doi: 10.1134/S1070427216110124.
7. Nikitin, A., A. Ozersky, V. Savchenko, I. Sedov, V. Shmelev, and V. Arutyunov. 2019. Matrix conversion of natural gas to syngas: The main parameters of the process and possible applications. *Chem. Eng. J.* 377:120883. doi: 10.1016/j.cej.2019.01.162.
8. Savchenko, V. I., A. V. Nikitin, Ya. S. Zimin, A. V. Ozerskii, I. V. Sedov, and V. S. Arutyunov. 2021. Impact of post-flame processes on the hydrogen yield in matrix partial oxidation reformer. *Chem. Eng. Res. Des.* 175:250–258. doi: 10.1016/j.cherd.2021.09.009.
9. ANSYS Academic Research CFD. CHEMKIN-Pro 15112. San Diego, CA: Reaction Design, 2011. CK-TUT-10112-1112-UG-1.
10. NUIGMech1.1 High T version. 2020. National University of Ireland Galway. Available at: http://c3.nuigalway.ie/combustionchemistrycentre/mechanismdownloads/ (accessed January 20, 2025).
11. Baigmohammadi, M., V. Patel, S. Nagaraja, A. Ramalingam, S. Martinez, S. Panigrahy, A. Mohamed, K. P. Somers, U. Burke, K. A. Heufer, A. Pekalski, and H. J. Curran. 2020. Comprehensive experimental and simulation study of the ignition delay time characteristics of binary blended methane, ethane, and ethylene over a wide range of temperature, pressure, equivalence ratio, and dilution. *Energ. Fuel.* 34:8808–8823.
12. Abd El-Sabor, Mohamed A., S. Panigrahy, A. B. Sahu, G. Bourque, and H. J. Curran. 2021. An experimental and modeling study of the auto-ignition of natural gas blends containing C_1–C_7 n-alkanes. *P. Combust. Inst.* 38(1):365–373.
13. C_1–C_{16} HT + Soot mechanism. Version 2003. CRECK Modeling Group, Politecnico di Milano. Available at: https://creckmodeling.chem.polimi.it/menu-kinetics/menu-kinetics-detailed-mechanisms/107-category-kinetic-mechanisms/411-mechanisms-1911-tot-ht-soot/ (accessed Janury 20, 2025).
14. Pejpichestaku, W., A. Frassoldati, A. Parente, and T. Faravelli. 2018. Kinetic modeling of soot formation in premixed burner-stabilized stagnation ethylene flames at heavily sooting condition. *Fuel* 234:199–206. doi: 10.1016/j.fuel.2018.07.022.

Received December 23, 2024
After revision January 9, 2025
Accepted January 16, 2025

Contributors

Bryukov Mikhail G. (b. 1963) — Candidate of Science in physics and mathematics, leading expert, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; mgbryukov@mail.ru

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

Troshin Kirill Ya. (b. 1949) — Doctor of Science in physics and mathematics, chief research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; troshin@chph.ras.ru

Vlasov Pavel A. (b. 1955) — Doctor of Science in physics and mathematics, chief research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; assistant professor, National Research Nuclear University MEPhI, 31 Kashirskoe Sh., Moscow 115409, Russian Federation; shocktube@yandex.ru

Arutyunov Vladimir S. (b. 1946) — Doctor of Science in chemistry, professor, chief research scientist, head of laboratory, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; chief research scientist, Federal Research Center for Problems of Chemical Physics and Medicinal Chemistry of the Russian Academy of Sciences, 1 Prosp. Academician Semenov, Chernogolovka, Moscow Region 142432, Russian Federation; professor, I. M. Gubkin Russian State Oil and Gas University, 65 Leninsky Prosp., Moscow 119991, Russian Federation; professor, Faculty of Fundamental Physical and Chemical Engineering, Lomonosov Moscow State University, Leninskie Gory, GSP-1, Moscow 119991, Russian Federation; v_arutyunov@mail.ru