COMPARISON OF THE EFFECT OF H_2O AND CO_2 ADDITIVES ON THE CONVERSION OF METHANE INTO SYNTHESIS GAS

A. R. Akhunyanov[1], P. A. Vlasov[1,2], V. N. Smirnov[1], A. V. Arutyunov[1], D. I. Mikhailov[1], and V. S. Arutyunov[1]

[1]N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation
[2]National Research Nuclear University MEPhI, 31 Kashirskoe Sh., Moscow 115409, Russian Federation

Abstract: For the first time, detailed kinetic modeling of the behavior of undiluted mixtures of methane with oxygen with CO_2 and H_2O additives was carried out taking into account the formation of microheterogeneous soot particles in the temperature range 1500–1800 K at a pressure of $P_{50} = 1$ bar. The appearance of soot particles was observed for rich mixtures, starting with the equivalence ratio $\phi = 3.33$. At the lower limit of the studied temperature range $T_{50} = 1500$ K, a small amount of soot particles (less than 1 %(mass) of C atoms) is formed, and they do not have a significant effect on the other parameters of the reacting system. A noticeable effect of soot particles at $T_{50} = 1500$ K is observed for $\phi = 8.0$. This is most clearly manifested in the fact that the temperature profile of the process changes markedly. When water is added, two maxima are observed on it at times of the order of 0.01 and 0.1 s. In the case of CO_2 additives, the second maximum is almost not pronounced. A complex temperature profile leads to the appearance of a second maximum concentration of hydroxyl OH radicals at ~ 0.1 s.

Keywords: methane conversion; syngas; CO_2 and H_2O additives; microheterogeneous soot particles; shock waves; detailed kinetic modeling

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Figure Captions

Figure 1 Simulations of changes in the concentrations of CH_4 (*1*), CO_2 (*2*), CO (*3*), H_2 (*4*), H_2O (*5*), and C_2H_2 (*6*) and temperature (*7*) at $T_{50} = 1500$ K, $P_{50} = 1$ bar, and $\phi = 8$ for mixtures with H_2O (*a*) and CO_2 (*b*). The temperature profile is also shown without taking into account the process of soot formation (*8*)

Figure 2 Simulations of changes in the concentrations of CH_4 (*1*), CO_2 (*2*), CO (*3*), H_2 (*4*), H_2O (*5*), C_2H_2 (*6*), and O_2 (*7*) and temperature (*8*) at $T_{50} = 1500$ K, $P_{50} = 1$ bar, and $\phi = 3.33$ for mixtures with H_2O (*a*) and CO_2 (*b*)

Figure 3 Simulations of changes in the concentrations of CH_4 (*1*), CO_2 (*2*), CO (*3*), H_2 (*4*), H_2O (*5*), C_2H_2 (*6*), and O_2 (*7*) and temperature (*8*) at $T_{50} = 1800$ K, $P_{50} = 1$ bar, and $\phi = 3.33$ for a mixture with CO_2

Figure 4 Simulations of changes in the concentrations of O_2 (*1*), O (*2*), and OH (*3*) for mixtures with additives of CO_2 (filled signs) and H_2O (empty signs) at $T_{50} = 1500$ K, $P_{50} = 1$ bar, and $\phi = 8$. Mixtures $0.5CH_4 + 0.375H_2O + 0.125O_2$ and $0.5CH_4 + 0.375CO_2 + 0.125O_2$ were used

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Contributors

Akhunyanov Artur R. (b. 1994) — research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; jkratos69@yandex.ru

Vlasov Pavel A. (b. 1955) — 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; assistant professor, National Research Nuclear University MEPhI, 31 Kashirskoe Sh., Moscow 115409, Russian Federation; iz@chph.ras.ru

Smirnov Vladimir N. (b. 1950) — 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; vns1951@yandex.ru

Arutyunov Artem V. (b. 1994) — Candidate of Science in physics and mathematics, research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; aarutyunovv@gmail.com

Mikhailov Dmitrii I. (b. 1994) — Candidate of Science in physics and mathematics, research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; mihalych2006@mail.ru

Arutyunov Vladimir S. (b. 1946) — Doctor of Science in chemistry, professor, 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; head of laboratory, 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; arutyunov@chph.ras.ru