Numerical study of H_2S-H_2O-air mixture conversion to hydrogen via activation of air by an electric discharge

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Hydrogen sulfide, which is a part of associated petroleum and so-called acid natural gases and which forms from the sulfur-containing fuels in petroleum refining industries, can serve as a source of hydrogen that is considered lately as an energy efficient and environmentally safe fuel. The direct conversion of H_2S to H_2 occurs only at rather high temperature, and such a process requires a fairly large amount of heat to be supplied to the system. For the implementation of low-temperature conversion of H_2S, an approach based on the partial oxidation of H_2S upon activation of the oxidizer (air) by an electric discharge is considered in this work.

Numerical study is carried out in an adiabatic flow reactor with the length of L=1 m at pressure P=1 atm and inlet gas velocity U_0=1 m/s, which corresponds to the gas residence time in the reactor of τ_r~1 s. Air, activated in an electrical discharge, and H_2S-H_2O mixture are supplied to the flow reactor inlet separately, where they mix and the homogeneous mixture moves in the reactor. Both flows are preliminarily heated up to the temperature T_0=500 K, the reduced electric field E/N in the discharge varies in the range of 1–150 Td (1 Td=10^{-17} V·cm²), the specific energy put into the discharge is E_s=0.3–0.5 J/ncm³, fuel-to-oxidizer equivalence ration was chosen to be ϕ=2, basing on the preliminary thermodynamic analysis, according to which, for such ϕ value, a maximum or close to the maximum yield of H_2 in H_2S-air mixture is realized.

Calculations have shown that a significant amount of H_2 is formed only after the H_2S-H_2O-air mixture ignites. At E_s=0.5 J/ncm³, the mixture with a fraction of water vapor $\varepsilon = n_{H_2O}^0 / n_{H_2S}^0$ =0–1 ($n_{H_2O}^0$ and $n_{H_2S}^0$ are the molar flow rates of H_2O and H_2S at the reactor inlet) ignites inside the reactor for any E/N value. But the shortest ignition length is realized for the discharge, producing maximum amount of $O_2(a^1\Delta_g)$ molecules. The values E/N~4–10 and 120–150 Td are most favorable. At E_s=0.3 J/ncm³, the mixture ignites only at ε=0–0.2 and only at the E/N values, when the molar fraction of $O_2(a^1\Delta_g)$ molecules is maximal. If the mixture ignites inside the reactor, H_2 yield does not depend on E/N. With an increase of the amount of H_2O in the mixture and a reduction of the energy E_s, supplied into the discharge, the range of E/N values, at which H_2S conversion occurs, narrows. On the other hand, the addition of water vapor leads to an increase of the relative yield of hydrogen $\delta = n_{H_2} / n_{H_2S}^0$ (n_{H_2} is the molar flow rate of H_2 at reactor exit) from 0.25 to 0.3 when ε varies from 0 to 1.