



Full Length Article

Super-adiabatic flame temperatures in premixed methane flames: A comparison between oxy-fuel and conventional air combustion



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ABSTRACT

As an alternative to usual combustion processes with air as oxidant, oxy-fuel processes are attractive in high temperature thermal or thermochemical processes, novel power plant concepts or in gasification processes. Especially for production of basic chemicals or synthetic fuels, high-purity synthetic gas without nitrogen dilution is required for further industrial processing.

In case of oxy-fuel combustion, the absence of nitrogen leads to higher flame temperatures and larger concentration of major species as well as intermediate species. In the present work, freely propagating methane-oxygen-nitrogen flames were numerically calculated using a 1D model from lean to rich conditions in order to investigate the appearance of super-adiabatic flame temperatures (SAFT). The calculations were performed for equivalence ratios of $0.5 < \Phi < 3.0$ with an increment of 0.1. Additionally, the nitrogen content of the oxidizer was varied from air to pure oxy-fuel conditions. Furthermore, the influence of preheat temperature and pressure on SAFT were analyzed for oxy-fuel flames.

The SAFT phenomenon was identified based on temperature and species profiles. Additionally, a detailed analysis of convection, diffusion and chemical source of both, temperature and species, were performed in order to investigate the role of physical transport processes on SAFT.

The results showed that the maximum flame temperature exceeds the equilibrium temperature for equivalence ratios $\Phi > 0.9$. Two different regimes were identified, where SAFT phenomenon appears. The first regime was found in slightly rich conditions ($1.0 < \Phi < 2.0$), whereas the second regime occurred in ultra-rich regime ($\Phi > 2.0$). A first maximum of temperature difference is observed at an equivalence ratio of $\Phi = 1.5$. Here, an exaggeration of approximately 120–180 K, depending on the applied reaction mechanism, was found for standard conditions. The first maximum at $\Phi = 1.5$ correlates with the maximum concentration of the H-radical, which plays a key role in the first SAFT regime. A minimum temperature difference of 50 K was identified at an equivalence ratio of $\Phi = 2.1$. While increasing the equivalence ratio further, the maximum flame temperature exceeded the equilibrium up to almost 400 K at $\Phi = 3.0$ in the second SAFT regime.

An increased preheating temperature enhanced the occurrence of SAFT in the first regime and degraded it in the second regime. Elevated pressure leads to the opposite effects with decreased SAFT in the first and increased SAFT in the second regime.

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1. Introduction

As an alternative to usual combustion processes with air as oxidant, oxy-fuel processes are attractive in high temperature thermal or thermochemical processes, novel power plant concepts or in gasification processes. Oxy-fuel processes provide significantly higher flame temperatures and exhibit advantages as increased thermal efficiency, higher processing rates, reduced flue gas volumes and the potential for reduced pollutant emissions at high oxygen concentrations [1]. Especially for production of basic chem-

icals or synthetic fuels, high-purity synthetic gas without nitrogen dilution is required for further industrial processing.

An interesting phenomenon in oxy-fuel combustion is the local appearance of super-adiabatic flame temperatures (SAFT) which has been identified and investigated in a few studies.

Meeks et al. [2] predicted in numerically calculated $C_2H_2/O_2/H_2$ -flames, that the local flame temperatures exceed significantly the adiabatic equilibrium temperature, even in case of including massive radiative heat losses of the gas phase in the calculations. The occurrence of SAFT in this flame was demonstrated experimentally via CARS spectroscopy by Bertagnolli and Lucht [3] and Bertagnolli et al. [4].

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Ruf et al. [5] recognized SAFT in rich premixed C_2H_2 - O_2 flames. Homogeneous calculation of the gas mixture showed an equilibrium H-concentration of 24%, whereas only 3% were experimentally detected. They proposed that the reaction $H_2 + M \leftrightarrow H + H + M$ is not fast enough in order to establish equilibrium at their boundary conditions.

Liu et al. [6] performed a systematic study of SAFT in premixed CH_4 /air-, different hydrocarbons/ O_2 - and H_2 / O_2 -flames. They showed that the occurrence of SAFT phenomena comes along with super-equilibrium concentrations of some hydrocarbon species and H_2O in the flames and results in a local temperature overshoot. It should be noted, that in premixed H_2 / O_2 -flames SAFT could not be detected.

Zamashchikov et al. [7] studied numerically super-adiabatic flame temperatures of CH_4 - and C_3H_8 -air in fuel-rich regime. The findings indicate that the degree of SAFT depends on the equivalence ratio, while the phenomenon occurs in rich regime. They proposed, that the diffusion of H_2 from the reaction zone to the preheat zone and its preferential oxidation is responsible for SAFT.

Liu and Gülder [8] analyzed the reaction flux in premixed CH_4 /air and CH_4 / O_2 -flames by artificially changing diffusion properties of H_2 and H radicals in their calculations. In contrast to [7], they concluded that the relative scarcity of H-radicals at the end of major heat release reactions and not the preferential diffusion of H_2 causes SAFT phenomenon. The H-radicals at high temperatures enhance the radical chain branching reaction $H + O_2 \leftrightarrow O + OH$. The reduction of the H-radical in the reaction zone is correlated to a temperature overshoot.

The effects of pressure and preheating on SAFT in rich premixed CH_4 /air flames were studied for equivalence ratios of $\phi = 1.4$ to $\phi = 1.8$ by Liu and Gülder [9]. Preheating leads to elevated combustion temperatures, which finally suppress a H_2O overshoot in the flame and hence, the SAFT phenomena. In pressurized systems, the degree of SAFT is enhanced.

Kumagami et al. [10] calculated laminar premixed CH_4 / O_2 / H_2 - O_2 -flames for fuel rich conditions under elevated pressures up to 3 MPa. They identified two different SAFT regimes: the first regime occurs for equivalence ratios of 1.0–2.0 and low water dilutions. The SAFT phenomenon gets less pronounced with increased pressure in the first regime, whereas it occurs in the second regime under all pressure conditions. Furthermore, it was shown, that the laminar burning velocity decreases with increased pressure for the first regime, whereas a slight increase with pressure was found under more fuel-rich conditions.

Takagi and Xu [11] showed numerically that SAFT is correlated by preferential species diffusion of H and H_2 in case of non-premixed combustion.

The literature review revealed that all studies focused on a small range of equivalence ratios and either on air or oxy-fuel combustion. The present study focuses on the SAFT phenomenon in gasification and oxy-fuel processes. Therefore, CH_4 - O_2 / N_2 flames are systematically investigated with established kinetics sets. Hereby, the oxygen-content of the oxidizer is varied from air to pure oxy-fuel combustion. All conditions were investigated for a wide range of equivalence ratios from $\phi = 0.5$ to $\phi = 3.0$ in order to exhibit global coherence.

Since industrial processes are operated with preheat and elevated pressure, their influence on SAFT is additionally analyzed in pure oxy-fuel flames.

2. Numerical approach

In the present study, the numerical calculations were carried out with the reactor for freely propagating premixed flames of the software package CHEMKIN 4.1. The PREMIX code was originally developed by Kee et al. [12,13].

The GRI 3.0 was used as a reference kinetic mechanism in the calculations [14], consisting of 53 species and 325 reactions. Additionally, the mechanism of Appel et al. [15] (99 species and 544 reactions) with detailed C_2 -pathway chemistry was used for selected cases. Unless otherwise stated, all presented results were carried out with the GRI 3.0 mechanism.

An initial grid of 24 points was used, which was adaptively refined to approximately 250 grid points. Grid independency was ensured in preliminary investigations. Full multicomponent and thermal diffusion were considered. A total reactor length of 10 cm was chosen for all calculations. The feed consists of CH_4 - O_2 / N_2 mixtures.

The comparison of air to oxy-fuel conditions were performed for standard thermodynamic inlet conditions (STC, 300 K, 1 atm). The oxygen content of the oxidizer was varied from 0.21 to 1.0 with an increment of 0.1. The flames were studied for a range of equivalence ratios of $0.5 < \phi < 3.0$ with an increment of 0.1.

Additionally, the oxy-fuel flames were calculated with three different inlet temperatures of 300 K, 500 K and 700 K, respectively, and the pressure was varied from 0.1 MPa to 1 MPa for $\phi = 1.0$ to $\phi = 3.0$ with an increment of 0.5.

3. Results and discussions

Since oxy-fuel combustion leads to significant higher flame temperatures and species concentrations than in air combustion, substantial dissociation and hence amount of radicals may be expected. Selected species of the H-O-system and the temperature in equilibrium state for methane-oxygen are presented in Fig. 1 for various equivalence ratios at standard inlet conditions.

The maximum equilibrium temperature is found at slightly rich conditions at equivalence ratios of $\phi = 1.0$ to $\phi = 1.2$. Here, the temperature varies in a range of approximately 3050 K only a few Kelvins. Those high temperatures lead to notable dissociation products. An amount of 8% molecular oxygen is found at stoichiometry and drops at an equivalence ratio of $\phi = 1.5$ below 1%. The peak of the O-radical (5%) and OH radical (10%) are located on the lean side, whereas the H-radical finds its maximum of 6.5% in rich conditions at an equivalence ratio of $\phi = 1.4$. Here, still an extremely high equilibrium temperature of 2973 K and subsequently large H-mole fraction are present and hence, a large diffusion flux of the H-radical may be expected due to high concentration and temperature gradients under those conditions.

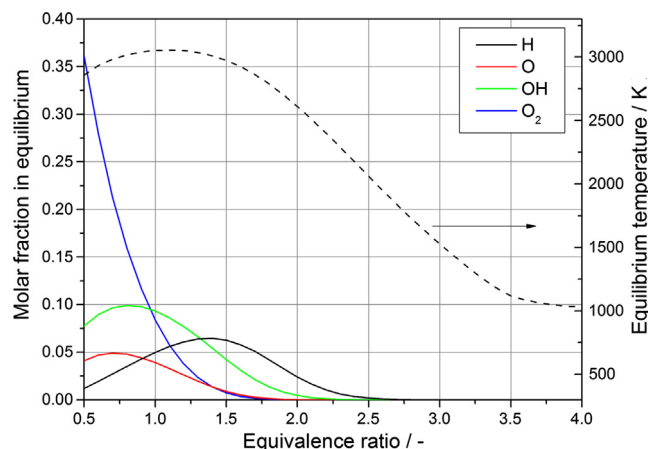


Fig. 1. Equilibrium temperatures and selected species at STC depending on equivalence ratio.

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