Entropy Generation and Exergy Loss in Natural Gas Mild Combustion Process

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1. Introduction

Recirculation of exhaust heat and gases in combustion chambers in which reactants are diluted with combustion products and temperature of reacting mixture is increased to above autoignition temperature, is a promising method to achieve high thermal (first law) efficiency and low emissions in advanced energy systems [1]. This combustion regime has been applied in different industries under terms such as “flameless oxidation” [2], “high temperature air combustion” [3], “moderate or intense low-oxygen dilution combustion” [4], and “diluted combustion” [5]. Widespread studies have been performed on this mode of combustion [1-9] and recently a comprehensive review has been also published [4]. Capabilities of this method in industrial burners have been proved by using gaseous, liquid and solid fuels [9] and application of this method in adiabatic combustion chambers such as gas turbine combustors is under development [10-12].

In order to fundamentally investigate the physics of different regimes in this mode of combustion, ideal reactors can be used. From application point of view, four basic cases are significant while all of them belong to flameless combustion category: HCCI (homogeneous charge compression ignition) [13], HBBI (homogeneous burnt backmixing ignition) [14], HCDI (homogeneous charge diffusion ignition) [15], and HDDI (hot diluted diffusion ignition) [16]. In previous studies, Soroudi and co workers have studied HBBI [17] and HCCI [18-22] homogenous regimes. This study focuses on combustion in HCDI and HDDI regimes. In the both later regimes, combustion has been investigated in counterflow flame configuration and molecular diffusion is also included due to non-homogeneity in the system. Counterflow flame as an interesting configuration for fundamental studies of combustion, has attracted our attention in the last few years [23-26].

Analysis of entropy generation and exergy loss is an effective way to evaluate second law performance and to minimize irreversibility in energy conversion systems. By using this method, it is possible to recognize contribution of transport processes and chemical reactions in local entropy generation and therefore optimize current or developing designs. Contrary to surveys concerning thermodynamic irreversibility in heat and mass transfer processes, there is less investigation on entropy analysis in combustion systems. Irreversibility in combustion system is a consequence of four processes: viscous dissipation, heat conduction, mixing or mass diffusion, and chemical reactions [27]. Recently, a comprehensive review on exergy analysis in combustion systems has been presented in reference [28].

The aim of this study is to investigate entropy generation and exergy loss in flameless combustion of natural gas. Among mentioned four basic cases, this study focuses on two non-homogenous ones, HCDI and HDDI, in order to perform a systematic analysis of molecular diffusion and chemical reactions irreversible processes. Exergy loss analysis of natural gas flameless combustion in counterflow configuration is reported in following.
2. Physical model

In this study, counterflow diffusion flame configuration was selected as the physical model. In this configuration two axisymmetric tubular nozzles lead two streams to enter flow field. Amount of fuel, diluent, and oxidant in these two streams change according to investigated conditions. All simulations were performed using CHEMKIN software package. Assuming that radial velocity changes linearly versus radius, the three dimensional flow field between two nozzles is reduced to a one dimensional case, because in this situation, fluid properties are a function of axial distance only. While using this 1-D model, changes in velocity, temperature, and chemical concentrations in the core of flow field between two nozzles can be estimated. It should be noted that in this condition, effects of corners are ignored. More details on governing equations and assumptions could be found in [29]. In this study, GRI-3.0 reaction mechanism [30] has been used to simulate natural gas combustion. This reaction mechanism comprises nitrogen chemistry and includes 325 elementary reactions and 53 chemical species. Further information about this mechanism and how to calculate chemical kinetics is described elsewhere [31].

In this section, entropy transport equation is defined and also method of calculation of exergy loss is presented. By using equations in the reference [27] and assumptions in references [32] and [33], general form of entropy transport equation is obtained:

\[
\frac{\rho Ds}{Dt} = \nabla \cdot \left( \nabla \left( \frac{\lambda\nabla T}{T} + \sum_k \nabla \left( \rho s_k D_{km} \nabla Y_k \right) \right) \right) + \left[ \frac{\tau \cdot \nabla \vec{V}}{T} + \frac{\lambda\nabla T \cdot \nabla T}{T^2} + R_\mu \sum_k \frac{\rho D_{km}}{X_k} \nabla Y_k \cdot \nabla X_k - \sum_k \frac{\mu_k}{T} \right]
\]  

(1)

In the above equation, \(\rho\), \(\tau\), \(\vec{V}\), \(s_k\), and \(\mu_k\) represent universal gas constant, viscous stress tensor, velocity vector, entropy of the \(k\)th species, and chemical potential of the \(k\)th species respectively. By using ideal gas assumption, chemical potential can be calculated according to the below equation:

\[
\mu_k = \bar{e}_k(T) - T \bar{s}_k^0(T) + R_\mu T \ln(\frac{X_k P}{P_{ref}})
\]  

(2)

In the above equation, \(\bar{e}_k\) and \(\bar{s}_k^0\) respectively represent molar internal energy of the \(k\)th species and molar entropy of the \(k\)th species at reference pressure (\(P_{ref}\)). Reference pressure is assumed equal to one atmosphere. In equation (1), the first bracketed right-side term is relevant to entropy transport rate. Terms in the second bracket correspond to entropy generation because of different physical processes. In the second bracket, terms are corresponding to entropy generation because of losses due to viscosity, heat conduction, mixing or mass diffusion, and chemical reactions respectively. Since entropy is a passive scalar, after solution of reacting flow field and finding the species, temperature, and velocity distributions in the domain, it is possible to determine the contribution of each of mentioned four processes in entropy generation by solving equation (1).

3. Numerical method

In the used software, discretization of governing differential equations is performed using conventional finite difference methods on a non-uniform grid. Diffusive terms become
discrete by using central difference and convective terms by forward difference scheme. However, it is possible to select central difference for calculation of convective terms in this software, but due to instability in solution processes it has been avoided and forward difference is considered as the default setting. Grid adapting in this software is controlled by adjusting CURV and GRAD parameters and in this study these parameters are set to 0.1. NPTS parameter controls the independency of solution from used grid and in this study is set to 150. By applying these values, solutions independent from the grid are obtained. Distance between two nozzles is assumed to be 2 cm in all cases. According to definitions in references [15] and [16], global strain rate is obtained by dividing inlet velocity of gases from the left nozzle by distance between two nozzles.

Velocities, temperatures, and chemical compositions of two streams of injected fluid from nozzles in the counterflow configuration determined the combustion regimes, i.e. HTCR (high temperature combustion regime), HDDI, AIDR (auto ignited deflagration regime), and HCDI. Details of investigated combustion regimes have been introduced in [15], [16] and [34]. Always the right-side nozzle is used to introduce high temperature gases (T_m = 1800 K) and the left-side nozzle is used for gases with ambient temperature (T_0 = 300 K). In nonpremixed regimes (i.e. HTCR and HDDI), air is introduced from the right-side nozzle and pure methane (X_f = 1.0 in HTCR regime) or methane diluted with nitrogen (X_f = 0.05 in HDDI regime) is introduced from the left-side nozzle. Global strain rate is always selected equal to 50 s^{-1} for nonpremixed flames. Therefore, it is possible to investigate effect of dilution on methane diffusion flame with high temperature air. In premixed regimes (i.e. AIDR and HCDI), always the right-side nozzle contains pure nitrogen and the left-side nozzle contains methane/air with different equivalence ratios (\varphi = 1.0 in AIDR regime and \varphi = 0.3 in HCDI regime). Global strain rate is always selected equal to 250 s^{-1} for premixed flames. In this way, it is possible to study effect of dilution on premixed combustion of methane with high temperature air. It should be noted that in all calculations pressure was set to atmospheric value and plug boundary condition assumption, in which gradients of properties on both nozzles are ignored, were applied.

4. Results and discussion

In figures (1) and (2), contribution of the four processes in entropy generation are plotted separately. Figure (1) is relevant to HTCR and HDDI regimes and figure (2) is concerning AIDR and HCDI regimes. According to figure (1), as the dilution become more intense, entropy generation decreases. In HTCR regime, entropy generation almost fairly divided into three parts which are results of mixing, heat conduction, and chemical reactions. Focuses of these processes are changing in different zones. As an example, contribution of chemical reactions in near flame front and proportion of heat conduction near maximum gradient of temperature are dominant. Contrary, in HDDI regime, entropy generation is a result of chemical reactions and heat conduction. Noticeable differences between entropy generations of the both premixed flames in figure (2) comparing to figure (1) are observed. The first point is that dilution in this condition has a stronger effect on decrease of entropy generation. Although in AIDR regime chemical reactions is the dominant contributor in entropy generation, by dilution and conversion of combustion mode to the flameless mode, contribution of chemical reactions in entropy generation in HCDI regime diminishes and heat conduction plays the major role in entropy generation in this condition.
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In other words, in high temperature diluted combustion of methane, either the HDDI nonpremixed regime or the HCDI premixed regime, main proportion of entropy generation is due to heat conduction.

Fig. 1  Entropy generation rate for HTCR (right) and HDDI (left) regimes

Fig. 2  Entropy generation rate for AIDR (right) and HCDI (left) regimes

Fig. 3  Percentage of exergy loss due to various processes in different combustion regimes

For better comparison, integral of rate of entropy generation in the domain has been calculated and by this means, exergy loss is evaluated in a global manner. The obtained
results are presented in figure (3) in form of percentage of exergy loss for each of the four processes respect to the exergy of the fuel. Due to inconsiderable contribution of viscosity in exergy loss, it has been removed from the plots in figure (3).

5. Conclusion

Local entropy generation and exergy loss in high temperature diluted combustion of natural gas in laminar counterflow configuration and in atmospheric conditions were investigated numerically. Various premixed and nonpremixed combustion regimes were studied. Results indicated that in both regimes, dilution effectively decreased total exergy loss. Because of dilution, contribution of conduction in entropy generation in both regimes has been maximized and contribution of chemical reaction and diffusion is reduced.

References

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