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Modeling of Oxy-Natural Gas Combustion Chemistry

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Two turbulence–chemistry interaction models that can be used in numerical modeling of oxy-natural gas flame combustion, where the reaction kinetics are fast and thermal dissociation in the products is of importance, have been compared and investigated. Detailed in-flame measurements, carried out in a coaxial jet diffusion flame of natural gas burning in pure oxygen, are presented and are used to validate the models. Both turbulent combustion models, namely, the presumed probability density function (PDF) model and the eddy dissipation concept (EDC), were combined with a chemical thermodynamic equilibrium procedure to describe the chemistry. The models differ in that, in the presumed PDF model, a statistical view point is utilized when calculating the local composition, whereas, in the EDC, the turbulent mixing rate plays a more dominant role. The calculations showed that, although the temperature field could be well predicted, the concentrations of intermediate species appeared too high. Similar predictions were obtained with both models, the largest differences were found in the flame sheet in the vicinity of the burner inlet. The much smaller influence of the description of the chemistry found in the flame calculations compared to that in the thermodynamic equilibrium calculations indicates that radiation has a strong smoothing effect on the results.

Nomenclature

a = parameter in the β function
b = parameter in the β function
$\tilde{f}$ = density-weighted probability density function
k = turbulent kinetic energy, m^2/s^2
Y_k^0 = mass fraction of species k in surrounding fluid
$\tilde{Y}_k$ = average mass fraction of species k
Y_k^* = mass fraction of species k in fine structures
γ^3 = fraction of fluid consisting of fine structures
ε = dissipation rate of turbulent energy, m^2/s^3
ν = kinematic viscosity, m^2/s
ξ = mixture fraction
ξ''^2 = mixture fraction variance
τ^* = mixing time in the eddy dissipation concept, s
χ = fraction of fine structures that can react
$\dot{\omega}_k$ = reaction rate of species k, 1/s

Introduction

COMBUSTION of natural gas with pure oxygen as an oxidizer has several advantages over conventional combustion. One of the most important advantages of the oxy-natural gas flame is the increase in combustion efficiency because no unnecessary N_2 has to be heated. Simultaneously, using oxygen instead of air has a dramatic influence on the flue gas composition. The flue gas will almost entirely consist of H_2O and CO_2. This strongly influences the radiative properties of the flame, and, combined with the high combustion temperatures that can be achieved, radiative heat transfer is greatly enhanced.

Numerical modeling of oxy-natural gas flames is a challenging task. Most of the turbulence–chemistry interaction models that can be used in the computational fluid dynamics (CFD) modeling of industrial processes are ad hoc models. Using these models in flames that are much hotter than conventional ones may lead to unexpected results, unless the models are thoroughly evaluated. The same also holds for the simplified models used to describe the kinetics of the combustion chemistry, for example, the kinetic expressions are usually developed and tested at much lower temperatures where the reverse reactions are of less importance.

At the high temperatures prevailing in oxy-natural gas flames, most of the chemical processes are extremely fast. It can, therefore, be assumed that the role of turbulent mixing as the rate-limiting process is more important in oxy-natural gas flames than in conventional natural gas flames. Simultaneously, the fast reaction kinetics imply that the reactions should be treated as reversible ones. With many of the proposed turbulence-interaction models describing the chemistry in such a way, this is not a trivial task. Hedley et al.[1] have modeled an oxy-natural gas flame with a four-step mechanism capable of accounting for thermal dissociation of CO_2 and H_2O. Unfortunately, in their paper they do not mention how the turbulence–chemistry interaction modeling was realized. Nevertheless, in oxy-natural gas flames the temperatures can be high enough for further thermal decomposition into radical species such as O, OH, and H to become significant. A reaction mechanism that can describe this in a realistic way has to be considerably more complex. The eddy dissipation concept (EDC)[2,3] is one turbulence–chemistry interaction model capable of handling such a description of the chemistry. This has been demonstrated in a number of studies.[4–7] However, although this is a feasible approach, the calculations are tedious. The other alternative is to apply equilibrium chemistry. This is, in general, considered to be a poor approach, but due to the significantly higher combustion temperatures that can be reached in oxy-natural gas flames, the kinetics of the reactions are faster than those in normal flames, and this might become a noteworthy alternative.

The purpose of this work was to investigate two models that can be used in numerical modeling of oxy-natural gas flames. These models use equilibrium assumptions to account for the importance of the fast backward reactions. In a separate thermodynamic equilibrium calculation, the influence of thermal dissociation was investigated. From the calculations it could be concluded that it is essential to include the most important radicals, that is, O, OH, and H. If these radicals are omitted the calculated combustion temperature will be significantly overestimated, which also influences the quality of the

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Table 1 Species included in the sets of thermodynamic data

Set I (32 species)	Set II (11 species)	Set III (8 species)	Set IV (6 species)
CH_4 CO_2 CO O_2 H_2O H_2 N_2 H O OH HO_2 H_2O_2 CH_2O HCO C_4H_2 C_3H_3 C_3H_2 CH_3 CH_3O CH_2OH C_2H_6 C_2H_5 C_2H_4 C_2H_3 CH_2CO C_2H_2 HCCO C_2H CH_2 CH_2* CH C	C_2H_6 CH_4 CO_2 CO O_2 H_2O H_2 N_2 H O OH	C_2H_6 CH_4 CO_2 CO O_2 H_2O H_2 N_2	C_2H_6 CH_4 CO_2 O_2 H_2O N_2

predictions of the main components. The effect of other radicals on the combustion temperature is much smaller. If no thermal dissociation is accounted for, the calculated combustion temperature will be far too high.

As a test case for mathematical modeling, an oxy-natural gas flame fired through a high-momentum burner is studied. The computational results obtained using the presumed probability density function (PDF) and the EDC are compared to measured ones. The results show that both models can be used to model oxy-natural gas flames. With the PDF model, the temperature in the hot reaction sheet in the mixing layer between the fuel and the oxygen jet were underestimated. Although this approach only requires that two scalars be considered, the predictions suffered from inaccuracies in the tabulation procedure. With the EDC, good agreement in the flow and temperature fields can be achieved, but the degree of dissociation is overestimated in the modeling.

Equilibrium Chemistry

To investigate the influence of thermal dissociation, radical species, the thermodynamic equilibrium temperature, and composition were calculated using four different sets of thermodynamic data. The species included in the different sets, labeled I–IV, are listed in Table 1.

In set I, 32 species were considered. In set II, apart from the species present in the fuel and the oxidizer stream, CO and H_2 as well as the most important radicals where included. In set III, the only additional species apart from those in the fuel and oxidizer were CO and H_2. In set IV, no additional species were included. In the investigation, the same fuel composition used in the description of the natural gas in the CFD modeling was used. Expressed as the molar composition, the composition of the fuel stream was 86% CH_4, 9.4% C_2H_6, 4.01% N2, 1.79% CO_2, and 0.21% O_2. The oxidizer stream was assumed to be pure oxygen. Figures 1 and 2 show the results from the calculations using sets II–IV. In Figs. 1 and 2, the results obtained with set I are not shown because the influence of additional radicals apart from O, OH, and H were negligible.

Figure 1 shows that the temperatures obtained with the set consisting of five species, that is, without allowing for any thermal dissociation, are unrealistic. The high temperatures on the fuel-rich side, that is, those where the slope of the temperature curve is negative, are only partly due to the neglecting of thermal dissociation. The main reason for the high temperature here is that without CO and H_2, the water shift reaction cannot be described. Using the set consisting of eight species (i.e., allowing for dissociation of CO_2 and H_2O into CO, H_2, and O_2) lowers the predicted temperature to 3378 K for a stoichiometric mixture. At this value of the mixture fraction, where the difference between the predictions is at its maximum, the inclusion of radicals into the calculation lowers the maximum temperature further, to around 3050 K.

In Fig. 2, the reason for the overestimation of the temperature on the fuel-rich side in the case when CO and H_2 are not included is clearly seen. It is also seen that although the difference in the temperature prediction between the cases where dissociation is accounted for is around 10%, the difference in the mole fraction CO_2 is as high as 35%. Consequently, including CO and H_2 in the combustion scheme can produce realistic temperature predictions, but the errors in the predicted compositions remain large.

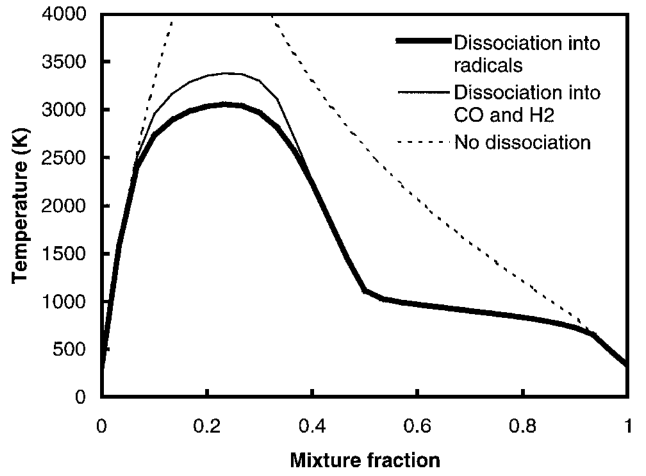

Fig. 1 Temperature as a function of mixture fraction obtained from thermodynamic equilibrium calculations.

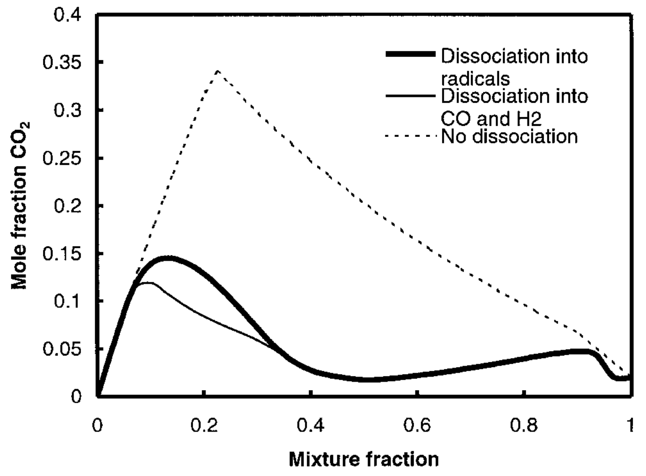

Fig. 2 Mole fraction of CO_2 as a function of mixture fraction obtained from thermodynamic equilibrium calculations.

Combustion Modeling

The numerical modeling of high-temperature flames is a challenging task. It should also be kept in mind that the most frequently used turbulence–chemistry interaction models have been assessed using measurements from studies of nonpreheated hydrocarbon–air diffusion flames where the chemistry is significantly different from that prevailing in oxy-natural gas flames. The aforementioned thermodynamic equilibrium calculations clearly show that accounting for thermal dissociation is of importance in these flames. This implies that the reactions should be treated as reversible ones. It is also desirable to include the dissociation into radicals such as O, OH, and H in the modeling. With many of the proposed turbulence-interaction models, describing such detailed chemistry is not a trivial task because this approach requires the use of a multiple-reaction-based description. On the other hand, at the high temperatures prevailing in oxy-natural gas flames, most of the chemical processes are extremely fast. That this, in turn, could motivate the reaction kinetics is totally neglected because it is then possible to use directly the thermodynamic equilibrium description. Here, at least two turbulence-interaction models can be applied in technical applications. One alternative is to use the presumed PDF model and the other is to apply the EDC.

The presumed PDF model is a well-established approach for turbulence–chemistry interaction modeling. The presumed PDF method tries to combine the advantages of the full PDF approach and the moment's approach. The basic principle is to use an approximate, but hopefully realistic, shape of the composition PDF, which can be described using only a few parameters.[8] The presumed PDF is often described with a function that can be characterized with two parameters. A popular function for describing the PDF is the β function, that is,

$$\tilde{f}(\xi) = \frac{\xi^{a-1}(1-\xi)^{b-1}}{\int_0^1 \xi^{a-1}(1-\xi)^{b-1}\,\mathrm{d}\xi} \tag{1}$$

The two parameters most frequently used to find the parameters needed to describe the approximate PDF are the mixture fraction ξ and the variance of the mixture fraction, ξ''^2. The mixture fraction can be defined from the starting point that, during chemical reactions, the chemical elements are conserved. The benefit of the presumed PDF is that its use is computationally favorable. It is not necessary to solve transport equations for the individual species because the composition is calculated using the presumed PDF. However, there are also limitations to this method; it is only applicable to diffusion flames and only one fuel and one oxidizer can normally be considered. Taking radiation into account also introduces some approximations into the method. For the nonadiabatic case, the assumption that the fluctuations in the mixture fraction are independent of the fluctuations in the temperature has to be made. With the presumed PDF model, two sets of thermodynamic data were used. In the first set 11 species were considered. The second set of thermodynamic data used with the PDF approach included 8 species.

The EDC model of Magnussen[2,3] is a general turbulence–chemistry interaction model that can be used for modeling premixed flames as well as diffusion flames. The case is not restricted to either type of flame, where only one fuel and one oxidizer is used. The model also allows for taking complex chemical phenomena into account, for example, a multistep mechanism for the description of the fuel oxidation. The EDC model is related to the eddy breakup model of Spalding[9] and the eddy dissipation combustion model of Magnussen and Hjertager,[10] but it is derived using a detailed description of the dissipative process in the flow. A complete description of the EDC model, as well as of its derivation, can be found in Refs. 2 and 3. The key feature of the models is that they discriminate between the reacting and the nonreacting part of the fluid. In the reacting part, it is assumed that the species are mixed on a molecular level and that the state can be obtained by solving a perfectly stirred reactor (PSR) problem. The model setup starts from the expression describing the dissipation of turbulent kinetic energy. From these expressions, a characteristic velocity scale and length scale for the turbulent structure where the mixing is completed are derived. These turbulent structures are in the EDC model referred to as fine structures. By the use of the velocity scale and length scale associated with the fine structures, an expression for the mass fraction they occupy is set up, that is,

$$\gamma^3 = 2.13(\nu\varepsilon/k^2)^{\frac{1}{4}} \tag{2}$$

The characteristic residence time in the fine structures is given by

$$\tau^* = 0.41(\nu/\varepsilon)^{\frac{1}{2}} \tag{3}$$

To obtain an expression for the mean average reaction rate, an expression for the mass transfer rate between the fine structures and the surrounding fluid is needed. This rate is usually modeled as γ^3/τ^*. The mean reaction rate for a species k can then be expressed as

$$\tilde{\omega}_k = (\gamma^3\chi/\tau^*)\left(Y_k^0 - Y_k^*\right) \tag{4}$$

The relation between the local mean value of the mass fraction of species k, its mass fraction in the surrounding fluid, and in the fine structures is

$$\tilde{Y}_k = \gamma^3\chi Y_k^* + (1-\gamma^3\chi)Y_k^0 \tag{5}$$

Within the fine structures, the species are assumed to mix on a molecular level. Thus, Y_k^* is obtained from solving a PSR problem, where the mass fraction of component k in the inlet is Y_k^0 and the residence time of the PSR is τ^*. If the reactions in the reacting part are assumed to be infinitely fast and reversible, the conditions in the PSR can be obtained through the thermodynamic equilibrium approach. In this study, the equilibrium composition was calculated using the program CEA[11,12] provided by NASA, which is based on an algorithm for the minimization of Gibbs free energy. With the EDC model, the thermodynamic data set with 11 species was used. Compared to the computational effort needed for solving a PSR problem with a reaction mechanism capable of accounting for dissociation into radicals, the computational effort needed for the equilibrium calculations is negligible.

Test Case and Modeling Setup

As a test case, a high-momentum nonswirling oxy-natural gas flame[13] fired in the IFRF furnace 2 was chosen. The internal length of the furnace was 3740 mm, and the dimension of the nearly square cross section was 1050 × 1050 mm. The chimney contraction diameter was 500 mm. The whole furnace was lined with refractory, giving a very hot flame. The natural gas entered through a round pipe in the center of the burner. The diameter of the fuel inlet was 16 mm. The oxygen stream entered through a 4-mm-wide annulus. The separation distance between the oxygen stream and the natural gas stream was 6 mm. The natural gas injection velocity was 105.4 m/s calculated on gas at normal temperature and pressure. The molar composition of the natural gas was 86% CH_4, 5.4% C_2H_6, 1.87% C_3H_8, 0.58% C_4H_{10}, 0.14% C_5H_{12}, 4.01% N_2, 1.79% CO_2, and 0.21% O_2. The inlet velocity for the oxygen stream was 109.7 m/s. The molar O_2 content of the oxidizer was higher than 99.5%.

The temperature was measured using a water-cooled suction pyrometer with a type B thermocouple.[13] The special feature of this suction pyrometer is the water cooling of the entire probe up to the tip, where the thermocouple is located. As a consequence, the gas was cooled before it reached the thermocouple. Therefore, it was necessary to calibrate the suction pyrometer using the nonintrusive coherent anti-Stokes Raman scattering (CARS) technique. With the broadband CARS technique it was possible to detect an entire N_2 Q-branch spectrum on a snapshot generated with a single laser pulse lasting about 10 ns. Because the spectral distribution of the Q-branch CARS spectrum displayed the population of the rotational and vibrational states, the temperature was determined directly from the spectrum. The temperature was derived by comparing the shapes of computed and experimental spectra. Single shot measurements were carried out with the repetition rate of the laser (10 Hz). Instantaneous temperature values measured at the same location were presented in a histogram, from which the temperature fluctuations were determined. The calibration of the pyrometer was carried out in an oxy-natural gas flame of 1-MW thermal input. Because the CARS measurement was performed with N_2 as an indicator molecule, it was necessary to add some nitrogen into the oxy-natural gas flame. The accuracy of the CARS temperature measurement was around 5% and, thus, the same measurement error is applicable to the suction pyrometer measurements. Also, the composition of the gas was measured using a sampling probe developed by the IFRF.[13] The dried and cooled gas was analyzed with a gas chromatograph. The NO_x content was determined using an analyzer working with chemiluminescence.

In the mathematical modeling an axisymmetric description of the furnace was used. The grid consisted of 208 × 96 cells, where the larger number of cells refers to the axial direction. All higher hydrocarbons were modeled as C_2H_6. The wall temperatures were set using measurement data. The turbulence was modeled with the standard k–ε model. Radiation was modeled with the discrete transfer method. A constant absorption coefficient of 0.3 was assumed for the gas. All calculations were made using the commercial code FLUENT, although the EDC, which is not found in FLUENT, was implemented as a user-defined subroutine. As an initial estimate for the calculations, results obtained with the IFRF combustion model[14] were used.

Results and Discussion

Figure 3 shows measured and predicted radial temperature profiles at the locations 0.22 and 1.42 m from the front wall. In the calculations, the thermodynamic data set with 11 species was used. Figure 3 also shows the corresponding information for the axial velocity component. The predicted temperature and velocity profiles agree fairly well with the measurements. The difference in the temperature predictions obtained with the different modeling approaches is small, except in the hot mixing layer between the fuel and the oxygen stream. This is also reflected in the velocity profile obtained with the PDF approach. In this region, the EDC seems to provide better results. The effect of including radicals in the CFD calculations was much smaller than the thermodynamic equilibrium study indicated. At $X = 0.22$ m, the results obtained with the 8- and 11-species setups were almost identical. At approximately $X = 1.0$ m, where the PDF approaches predicted the highest temperature, the difference was at its maximum. Here, the 11-species setup predicted a temperature of 2450 K, whereas the 8-species setup predicted a temperature of 2530 K. According to Fig. 1, the difference in the adiabatic combustion temperature obtained with these two sets of thermodynamic data is over 300 K. The much smaller difference obtained in the CFD calculations indicates a smoothing effect of radiation on the predictions.

A more severe test of the quality of the predictions is to compare measured and predicted species concentrations. Figure 4 shows the radial distributions of CO_2, CO, and H_2, obtained using the 11-species setups, at $X = 0.22$ and 1.42 m from the front wall. In the predictions of the CO_2 concentrations, the EDC provided excellent results at the location closest to the burner, that is, at $X = 0.22$ m. Farther downstream the scatter in the measurements makes the results more difficult to evaluate, but the predicted CO_2 level away from the centerline agrees with those measured in the flue gas. With the presumed PDF model, the CO_2 level in the vicinity of the centerline was much lower. The CO_2 level is also slightly lower farther away from the centerline. The reason for this discrepancy was examined in some detail. It was found that the mixture fraction calculated from the concentration field obtained with the EDC agreed closely with the mixture fraction calculated with the PDF approach. The source of the discrepancy was to be found in the table the concentrations were retrieved from in the PDF approach. The PDF model was calculated with the version of the model found in FLUENT. Although the highest possible resolution allowed by the software was used when tabulating the concentrations as a function of mixture fraction, mixture fraction variance, and enthalpy level, the strong nonadiabatic effects made the accuracy of this table insufficient. Effects of the inaccuracies in the tabulation procedure could also be observed when comparing the result obtained with the 11- and 8-species setups. Here, a slight difference in the O_2 concentrations of the flue gas leaving the combustor could be observed, although only negligible amounts of dissociation products were present. Nevertheless, note that the mole fractions are reported on dry bases. Because the flue gas consisted to more than 60% of H_2O, the difference is accentuated.

Not only were the concentrations of the stable combustion products determined during the experiments, but H_2 and CO were also measured. Figure 4 also shows the measured and predicted profiles of CO and H_2. The quality of the CO and H_2 predictions at $X = 0.22$ m is difficult to judge because of the very steep profile. Although the levels at the sampling locations are in reasonable agreement, it is likely that the CO and H_2 levels are significantly overestimated in the predictions with both the PDF approach and the EDC. At $X = 1.42$, the quality of the CO predictions obtained with the EDC model is better than those obtained with the PDF approach, although the predicted concentrations are clearly higher than the measured ones. At the same location, the PDF approach gives superior results to the EDC regarding the H_2 level. In the examination of the CO_2 prediction obtained with the PDF model, the accuracy of the tabulation procedure was found insufficient. As a consequence, the quality of the agreement in the H_2 predictions obtained with this model must be judged carefully.

The presumed PDF model is potentially less computationally demanding. However, in the present study, the presumed PDF model proved at least as difficult and tedious to use. As a result, the only slightly more computational expensive EDC seems to be a useful alternative. The EDC also does not suffer from the limitations imposed

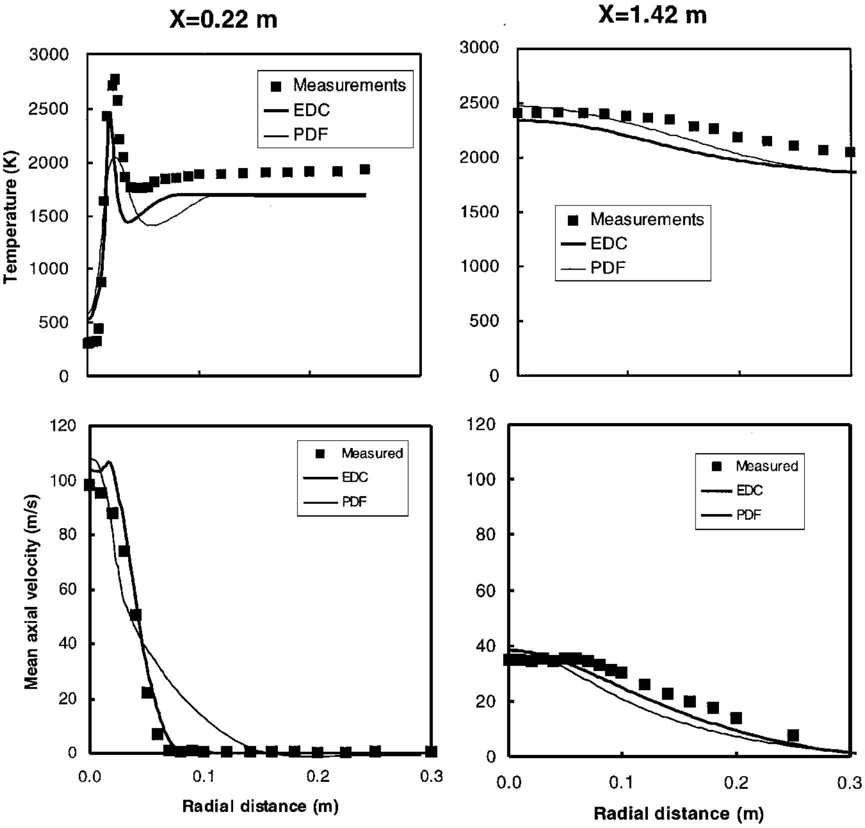

Fig. 3 Measured and computed radial temperature profiles and axial velocity profiles at X = 0.22 and 1.42 m.

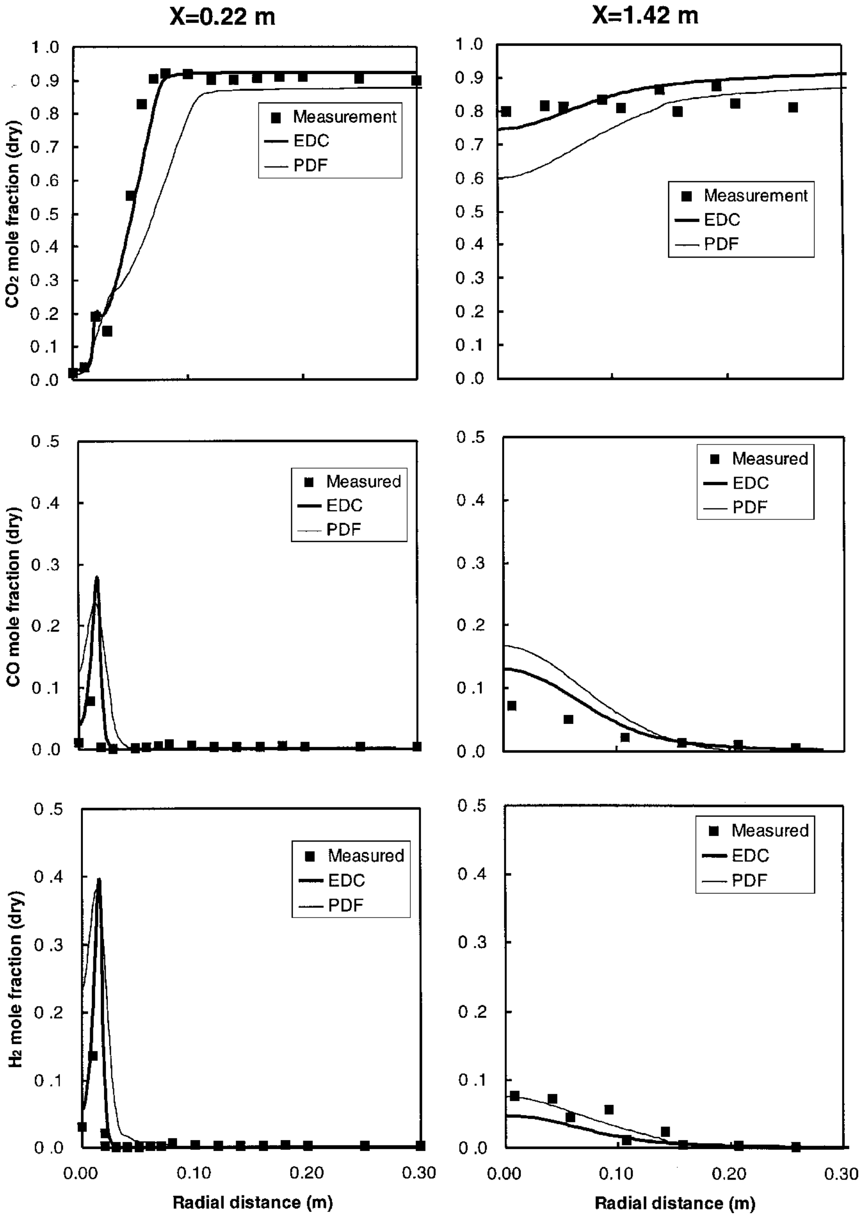

Fig. 4 Measured and computed profiles of CO_2, CO, and H_2 at $X = 0.22$ and 1.42 m.

by the use of the mixture fraction–mixture fraction variance concept. The very high H_2 and CO levels obtained inside the flame compared to the measure levels suggest that accurate predictions cannot be obtained without accounting for the reaction kinetics.

Conclusions

Two turbulence–chemistry interaction models (i.e., the presumed PDF model and the EDC), which together with the thermal equilibrium description of the chemistry are able to account for thermal dissociation in oxy-natural gas flames, have been studied. Both models have similar capabilities to predict temperature, concentrations, and flowfield in such high-temperature processes.

The presumed PDF model suffered from inaccuracies in the tabulation of the fluid state as a function of mixture fraction, mixture fraction variance, and enthalpy level. As a consequence, the predictions obtained with the EDC were in better agreement with the measurements. However, the predicted concentrations of H_2 and CO in the flame were generally higher than measured ones and appeared unrealistic. It seems that accurate prediction even in the high temperatures prevailing in oxy-natural gas flames requires that reaction kinetics be taken into account.

The separate equilibrium calculations of the adiabatic combustion temperature, using sets of thermodynamic data consisting of a different number of species, show the importance of taking intermediate combustion products into account. An accurate result also depends on the inclusion of the O, OH, and H radicals. However, the much smaller influence of the description of the chemistry found in the flame calculations compared to that in the thermodynamic equilibrium calculations shows that radiation has a large smoothing effect on the results.

In the oxy-natural gas flame the presumed PDF model is almost as computationally expensive as the EDC model due to convergence problems caused by the tabulated data. The prediction obtained with the EDC was also in better agreement with the measurements. As a result, the only slightly more computationally expensive EDC seems to be a better choice. The EDC also does not suffer from the limitations imposed by the use of the mixture fraction–mixture fraction variance concept. Finally, with EDC, reaction kinetics can be taken into account, although this would greatly increase the computational expense of the model.

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