RADIATION AND SOOT FORMATION IN A TURBULENT DIFFUSION FLAME

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In most of the flames, radiative transfer significantly modifies the temperature field and hence the concentrations of reactive species. On the other hand, the radiative power field strongly depends on the temperature and on the composition of the medium. In diffusion flames, for which combustion occurs in a large range of mixture ratios, including zones above stoichiometry, a large amount of soot particles is produced, which strongly enhances the radiative transfer. Therefore, there is a strong coupling between combustion and radiative transfer, mainly through the highly nonlinear dependence of these phenomena on temperature. In numerical simulations, this coupling can be treated by an iterative procedure.

MODELING

The convergence of the coupled aerothermochemistry, soot formation and radiation calculation is obtained by an iterative procedure. Each iteration includes the following steps.

(i) The first step consists in an aerothermochemical Reynolds Averaged Navier-Stokes calculation, based on a given field of radiative source term. The averaged balance equations of global mass, momentum, energy, masses of the five main chemical species O_2, N_2, C_2H_4, CO_2 and H_2O and of all the scalar quantities involved in the turbulence model are solved. A standard $k-\varepsilon$ model is used. A conventional model of turbulent combustion is used. It is based on the assumption of fast chemistry.

(ii) The second step consists in a Lagrangian calculation of the soot volume fraction, based on the averaged quantities computed in the first step (i). The chemical kinetics involves 37 species and 113 reactions[1]. A five-equation soot model is used. The five soot parameters are respectively the light and heavy soot precursor concentrations, the soot volume fraction, the number of soot particles per volume unit and the total surface of soot particles per volume unit. This model accounts for the phenomena of nucleation, surface growth, coalescence and oxidation. With an adapted statistical treatment of the fluid particles, the calculation of the joint Probability Density Function of the reaction progress variable, the mixture ratio and the soot volume fraction allows accounting for Turbulence-Radiation Interaction (TRI) in the next step (iii).

(iii) The third step consists in a radiative transfer calculation which leads to a new field of radiative source term to be used in the first step (i) of the next iteration. The radiative source term, also called radiative power, is calculated by a Monte Carlo method[2]. The reciprocity principle is used to calculate the radiative power exchanged between the origin cell and all the other cells crossed by an optical path. TRI modeling[3] is based on the partition of all the optical paths into a succession of independent coherent turbulent structures supposed to be homogeneous and isothermal. The radiative properties of these structures are randomly obtained from the joint PDF calculated in the second step (ii). The local size of a turbulent structure is equal to the local turbulent integral length. The spectral absorption coefficient of the gas mixture is given by a CK model[4] .The spectral absorption coefficient (in m^{-1}) of the soot particles is equal to $550\,\nu\, f_V$, where ν is the wavenumber in cm^{-1} and f_V the soot volume fraction. Radiation scattering by soot particle aggregates is not considered.

In order to prevent an oscillatory behavior in the iterative procedure and to speed up the convergence, the radiative source term is under-relaxed by averaging the results of two consecutive radiative transfer calculations after the second iteration.

APPLICATION TO A TURBULENT DIFFUSION FLAME

The considered flame is a turbulent ethylene-air diffusion jet flame[5]. The iterative procedure has been completely achieved with two different assumptions for the radiative transfer calculation: i) without and ii) with TRI. In both cases, the convergence is reached after 7 iterations. In the case without TRI, the total radiative heat loss at convergence amounts to 33% of the combustion heat release. With TRI, the corresponding value is 41%. The TRI effect is an increase by 22% of the radiative heat loss. It is worth noticing that this relatively small increase is due to compensation between large increases of the total emitted power by 44% and of the total absorbed power by 74%. In fact, a larger fraction of the radiative emission is self-absorbed in the flame with TRI (43%) than without TRI (35%). These two values prove that the assumption of optically thin medium is not valid in this flame.

The increase of the total power emitted by the flame is mainly explained by the non-linear temperature dependence of the equilibrium spectral intensity, which results in a higher radiative emission in the presence of temperature fluctuations than without fluctuations. The increase of the absorbed power is partly due to the increase of the emitted power, but also to a stronger correlation between emission and absorption with TRI than without TRI. In TRI modeling[3], the spectral radiative properties used to calculate the absorption are constant along a whole crossed turbulent structure. In this structure, the spectral absorption coefficient is large if the structure center is located in a place where the soot and absorbing gaseous species concentrations are high, whatever the concentrations in the other points of the structure. Since the size of a turbulent structure is generally larger than the mesh size, the emission-absorption correlation gives rise to a higher self-absorption than without TRI. The effect of the turbulent structure size on the power self-absorbed in the flame has been studied[3]. As expected, it has been found that the absorption decreases when the turbulent structure size decreases. When the turbulent structure size is sufficiently small, the results tend to those obtained with the Optically Thin Fluctuation scale Assumption.

Figure 1 shows that the highest absolute values of the radiative power with TRI are comparable to those without TRI, but the emitting zone is wider with TRI than without TRI. Moreover, the strongly emitting zone is shifted downstream when TRI is considered. The TRI effect on radiative power can be locally very strong. For example, at $r \approx 2\,\mathrm{cm}$, taking into account TRI increase the absolute value of the radiative power by about 100%. Near the flame front, on the air side, the average temperature decreases when the distance to the axis increases and, without TRI, the emitted power decreases rapidly. With TRI, a state of relatively low average temperature can be characterized by successive instantaneous states of very low temperature and relatively high temperature. Due to the non-linear temperature dependence of the equilibrium spectral intensity, these conditions are favorable to the radiative emission. Consequently, the emission zone is wider with TRI than without TRI. It is worth noticing that, due to the axial symmetry, the points located far from the axis have a stronger impact on the total radiative heat loss than the points located near the axis. That is why, when TRI is considered, the total radiative heat loss increases, while the highest absolute values of the radiative power decrease.

Due to a higher radiative heat loss value, the average gas temperature is slightly lower when the TRI is considered, as shown in Figure 2. The axis temperature obtained with TRI is 70 K lower than without TRI. The global amounts of soot in the flame obtained in both cases are close: $1.77\ 10^{-6}$ kg without TRI and $1.84\ 10^{-6}$ kg with TRI. The slightly higher soot level with TRI is explained by a lower oxidation rate due to a lower temperature in the second half of the flame.

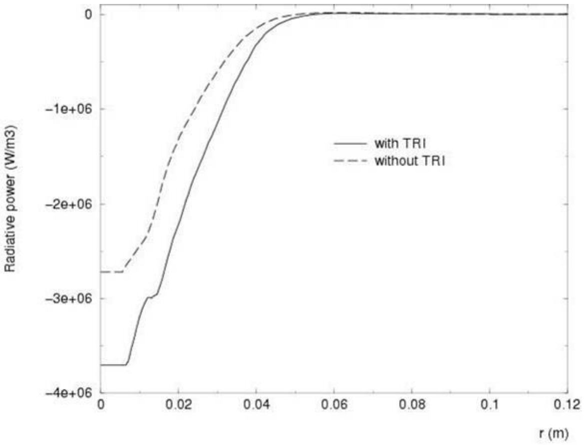

Figure 1: radial profiles of radiative power at 1 m above the burner

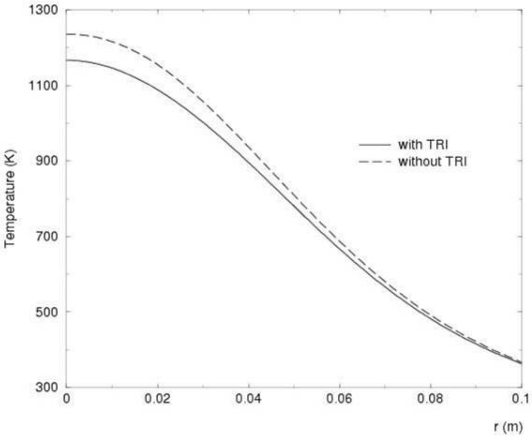

Figure 2: radial profiles of temperature at 1 m above the burner

CONCLUSION

An iterative coupled procedure involving a Reynolds Averaged Navier-Stokes calculation, a Lagrangian calculation of soot formation and a Monte Carlo radiative transfer calculation has been applied to a turbulent diffusion sooty flame with a very large radiative loss. This procedure converges after about 7 iterations. The calculation, during the Lagrangian step, of the joint probability density function of the reaction progress variable, of the mixture ratio and of the soot volume fraction allows accounting for the interaction between turbulence and radiation. This interaction increases the radiative heat loss by more than 20%. The effects of this interaction are important in the second half of the flame: it results in a 70 K temperature decrease on the flame axis at 1 m from the ethylene inlet. The fraction of the emitted radiation self-absorbed in the flame is large, especially when the turbulence-radiation interaction is taken into account. In that case, nearly 40% of the emitted radiation is self-absorbed in the flame. This is a consequence of the strong correlation between the emission and absorption properties in the turbulent structures located in the emitting zones.

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