Experimental and numerical investigation of radiation in oxyfuel combustion

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Abstract

Radiative heat fluxes are measured in a lab scale test rig. Numerical simulations of a virtual gas turbine combustor are performed using several spectral radiation models, in addition the effect of different numerical radiation models have been tested on a gas turbine combustion chamber. It was shown that the effect of radiation in oxyfuel combustion is very strong compared to air-fired systems. Numerical simulations showed that a spectral model is needed for an accurate prediction of wall heat fluxes in an oxyfuel gas turbine combustor.

Keywords: CO2, oxyfuel, radiation

Introduction

The oxyfuel concept is a promising technology for pre-combustion CO_2 capture since the ideal combustion of a stoichiometric mixture of hydrocarbons and oxygen theoretically results in a flue gas consisting solely of the combustion products H_2O and CO_2. In order to lower the extremely high temperatures associated with stoichiometric oxygen combustion, a part of the CO_2 stream is recycled. This strongly affects the combustion characteristics. Due to the high temperatures and CO_2 concentrations, radiative heat transfer is expected to play a more important role in oxyfuel processes compared to conventional air combustion systems, leading to increased radiative wall heat fluxes and higher wall temperatures. The temperature of the combustor walls is a critical parameter for the design of a combustor since it is limited by the properties of the material and has large impact on the combustor lifetime. Hence, an accurate prediction of radiative heat transfer is mandatory for the design of an oxyfuel combustor.

Experimental investigations

The experimental set up consists of a confined non-premixed flame. The burner provides a circular jet of methane into a circular co-flow of air or O_2/CO_2. The ratio of O_2 and CO_2 in the co-flow can be varied. The radiative heat flux is measured by a calibrated probe located on the combustion chamber wall, and emission spectrum of the flame at 60 mm above the nozzle exit is measured by a spectrograph imager. Experiments have been achieved for a constant co-flow velocity and varying Reynolds number flames.

The left plot in Figure 1 shows the axial flame flux density profiles at Re = 900, corresponding to a 2 kW flame, with three different oxidant compositions, i.e. air and O_2/CO_2 mixtures with molar ratios of 40/60 and 50/50. It is observed in the left hand plot of Figure 1 that the near field radiative properties of the flame is very dependent on oxidant composition. Both the total heat flux radiated and peak value position are influenced. By increasing the O_2 content, the adiabatic temperature and stoichiometric mixture fraction vary leading to variation in the flame structure. The flame shortens as O_2 increases as a consequence of the latter effect. The higher intensity of the heat flux can be explained partly by the increase in temperature, but also partly by the change in local species concentrations. Indeed, not only increases the concentration of radiating gas (CO_2, H_2O and CO) with O_2 enrichment, but also the soot volume fraction as a consequence of increased temperature on the local chemistry.

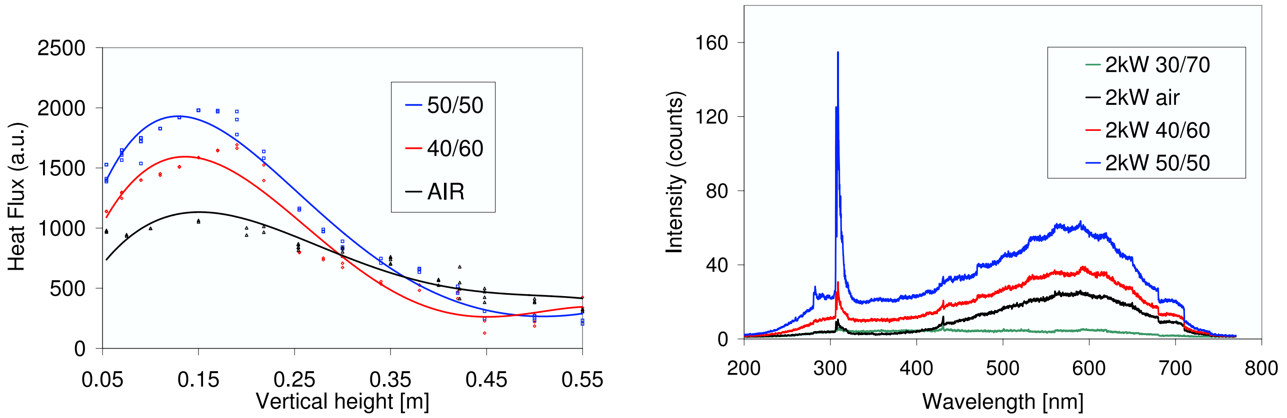

Figure 1: Radiative heat flux distribution along the flame axis (left) and emission spectra (right) of a jet flame (Re = 900) burning in different oxidant atmospheres.

The near field emission spectra of the right hand plot of Figure 1 are taken at the same conditions as those of the left hand plot of the same figure, plus one case at 30% O_2. The continuous broadband signal in the visible region of the spectrum is attributed to soot emission and is seen to increase considerably with O_2 content in the oxidant. Several sources contribute to this effects: first the increase in temperature on the black body radiation law; the increase in local soot volume fraction due to temperature increase; the decrease in CO_2 concentration in the oxidant gas layer with its accompanying reduction in absorption; and finally the blue shift of the peak wavelength black body radiation of soot with increasing temperature according to Wien's law, which displace the soot black body radiation from the strongest absorbing lines of CO_2 in the IR. Remarkably enough the case with 30% O_2 shows very low broadband intensity as compared to the air case, even though both flames have similar adiabatic temperature. It is believed that the radiative loss due to the very high concentration of CO_2 locally decreases the temperature to a point where the soot formation mechanism is inhibited. This point needs however further investigation.

In the far field of the flames investigated, the heat flux reach the same levels for all flames. It is known that the increased local soot volume fraction accompanying an increase in oxygen concentration is compensated by an increased oxidation rate of soot downstream the flame, attaining global soot levels that are in fact lower than in the air case [1].

Numerics

Depending on application, need for accuracy, computational resources available and dimensions of the problem, there are several approximate methods for solving the radiative transfer equation (RTE). In the following we have chosen the discrete ordinates method (DOM) with 24 different directions.

Model	ref	Formalism1				Formalism2			
		Name	abbr.	bins	S	Name	abbr.	bins	S
WSGG	[2]	Grey	WSGG1	1	1	Non-Grey	WSGG3	3	4
WBCK	[3]	Rest. mult. gas	RMF3	3	7	Spectral	SPF19	19	258

Table 1: Summary of the different models handling the radiative properties of gases, together with specifications of the different formalisms used. Here bins means number of absorption bins, while S is the required CPU time (in non-dimensional units).

For oxyfuel combustion it is crucial to solve for the frequency dependency of the gas. This can be done in many ways, for example by splitting the spectrum into a large number of frequency bins, and then solve the RTE for each of these bins. Since the absorption lines generally are very thin, the required number of bins are very large, which makes this method unsuited for industrial applications.

The aim of the current survey is to find which of the available methods that resolved the problems related to the radiative properties best, at the same time as we want to emphasize on the importance of solving the radiation properly in oxyfuel combustion. As there is a relatively large number of available methods, we have chosen two of the most promising ones; the Weighted Sum of Grey Gases (WSGG) of Smith et al. (1982) [2] and the Wide Band Correlated-K (WBCK) of Denison and Fiveland (1997) [3]. Both methods have different formalisms which take care of the radiative properties in different ways. The most accurate is the spectral formulation (SPF19) where we solve the RTE for 258 individual frequency bins using the WBCK model, but as this is a very expensive formalism we have also looked at less resource demanding models like the restricted multiple gas formalism (RMF) and the grey and non-grey WSGG formalisms. In the RMF and WSGG3 formalisms, the spectrum is discretized in absorption coefficient space, instead of frequency space, in order to reduce the number of RTE's to be solved. The WSGG1 formalism have no spectral treatment at all. One absorption bin corresponds then to one absorption coefficient interval. In the RMF, absorption bins for H_20 and CO_2 are solved individually, whereas in the WSGG formalisms the absorption bins are common for H_2O and CO_2. The latter is only valid for a spatially constant ratio of H_2O and CO_2, which is not the case in oxy-fuel combustion. The WSGG model is the standard model used in most commercial CFD tools. For more details on the different formalisms see Ströhle (2003) [4]. A summary of the models and formalisms used is found in Table 1.

We have used the in-house CFD code SpiderII for all radiation models. In addition to the radiation models we have also solved the incompressible Navier-Stokes equations together with a $k-\epsilon$ model for the turbulence, an eddy dissipation concept (EDC) model for the species and an enthalpy equation for the energy.

Virtual combustor

In order to extract the effects of the species composition in a gas combustor we look at a virtual gas combustor, which is approximated by a rectangular enclosure with the dimensions of $L_x \times L_y \times L_z = 0.4\text{m} \times 0.2\text{m} \times 0.2\text{m}$. The temperature and concentration profiles are held constant, and all other processes other than radiation are neglected. At $x = 0$ the gas in the center consist of a stoichiometric fuel/oxidizer mixture, and the gas close to the wall consists of the diluent. The fuel/oxidizer mixture is assumed to react linearly in x until it is completely reacted at $x = L_x/2$.

Three different cases are considered, i.e. a conventional combustor with air as an oxidizer (Case 1), and two oxyfuel cases with O_2 as an oxidizer and CO_2 as a diluent, where the CO_2 mole fraction of the fuel is 0.4 for Case 2 and 0.625 for Case 3, and the CO_2 mole fraction of the diluent is 1 for both case 1 and 2. The temperature of the fuel/oxidizer mixture is set to 700K.

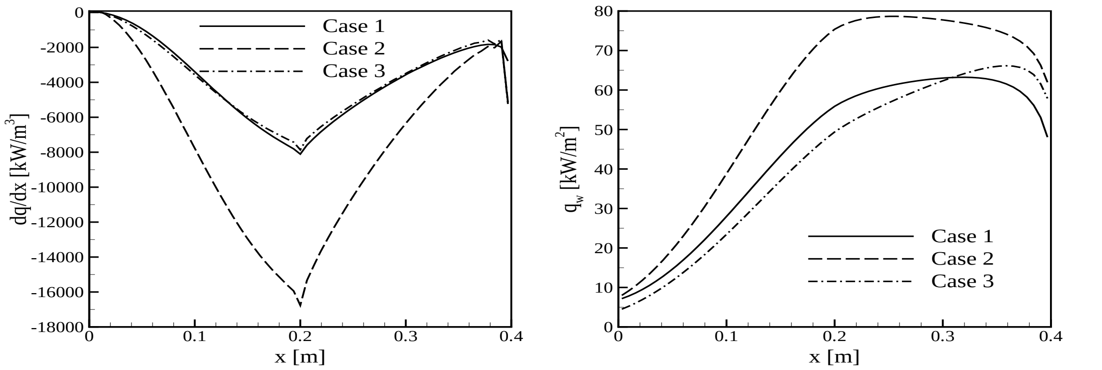

Figure 2: Reference calculation, using SPF19, of radiative source along combustor centerline (left) and radiative flux along a line on the wall (right) for three cases of a virtual gas turbine combustor.

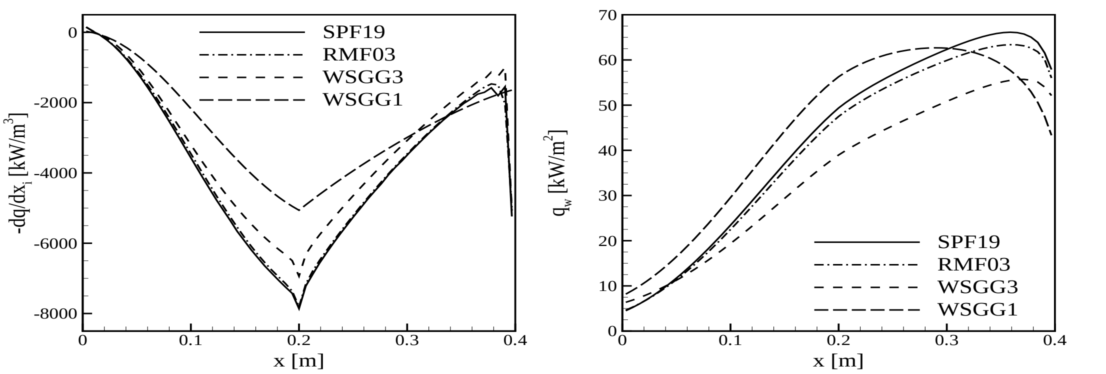

Figure 3: Radiative source (left) and radiative flux (right) for case 3 comparing three different models; the spectral formulation of WBCK with 19 absorption bins, corresponding to 258 frequency bins (solid line), the restricted multiple gas formulation of WBCK with 3 absorption bins (dashed-dotted line), the non-grey formulation of the WSGG with 3 absorption bins (dashed line) and the grey formulation of the WSGG with 1 absorption bin (long dashed line).

The results of the WBCK-SPF19 are used as a reference since it is the most accurate approach in this test. The computed radiative source along the centerline and the radiative fluxes along a line on the wall for the three cases using the SPF19 are shown in Figure 2. The radiative source of Case 2 is more than twice as large as the other two cases due to much higher maximum temperatures, the flame temperatures are 2627K, 3564K and 2510K for case 1, 2 and 3 respectively. The radiative source of the other cases is almost the same, although the maximum temperature of Case 3 is lower than that of Case 1, which can be contributed to the higher CO_2 concentrations in the oxyfuel case. The radiative wall heat flux is also highest for Case 2. However, the differences are much smaller due to the large amount of re-absorption by CO_2 in the oxyfuel cases.

In Figure 3 we plot the radiative source and radiative flux for case 3 calculated with different radiation models. The solid line correspond to the SPF19, which is used as a benchmark for the other models. Looking at the radiative source we see that the WBCK with the restricted multiple gas formulation and 3 absorption bins (RMF3) is in excellent agreement with the benchmark. This is to some extent also true for the radiative flux, although the agreement is slightly less here. Looking however at the weighted sum of grey gases (WSGG1) we see that the agreement is much worse even when we use a non-grey formalism with 3 absorption bins (WSGG3). The same tendencies as we see here are also present for case 2.

Looking at the required CPU times for the different models in Table 1 it seems to be a good compromise between accuracy and speed to use the RMF3 formalism. In addition to the formalisms presented here we have also run similar tests with other formalisms of the WBCK model, but they gave less favorable compromises between speed and accuracy.

Gas turbine combustor

Numerical simulations of a GE/SNECMA CFM56 turbofan engine have been performed [1]. The annular gas turbine combustion chamber is periodic with 20 fuel injectors, so just a single 18° sector of the flame tube is considered. Within the sector where the calculations are conducted, there are five dilution holes on the curved top and bottom surfaces. There are also seven and six film cooling slots on the top and bottom surfaces respectively. A swirler cup for fuel injection as well as a splash plate is situated just before the inflow boundary. A more detailed description of this configuration can be found in Gran (1994) [5]. A stoichiometric mixture of fuel and oxygen, diluted with 25% recycled gas (mainly CO_2), is injected at 35 bar through the swirler cup, while recycled gas is injected through the other inlets.

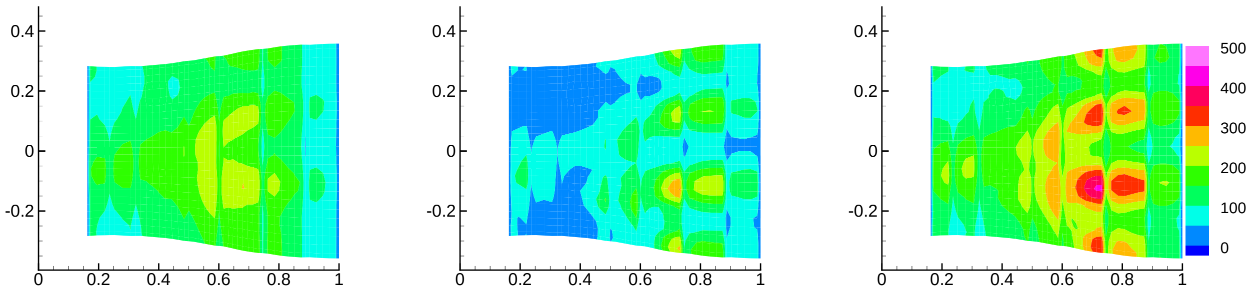

Figure 4: Radiative heat flux [kW/m^2] on bottom wall of combustor calculated with the WSGG1 (left), WSGG3 (center) and WBCK-RMF3 (right) formalisms.

The radiative wall heat flux on the lower wall of the combustion chamber is shown for three different models in Figure 4. The models shown are the WSGG1 (left), the WSGG3 (center) and the WBCK-RMF3 (right). The vertical lines in the four plots are due to the six cooling slots on the bottom wall.

Since we do not have experimental data to compare with we do not know which of the three approximations is the most accurate, but from previous work we believe the WBCK-RMF3

[1]The reason for choosing this particular gas turbine combustor was that the numerical grid was already available beforehand.

approximation to be the most accurate of the three. This assumption is also supported by the fact that this formalism is the on of the three that is most careful with the spectral handling. Comparing the two latter panels of Figure 4 we see that the WSGG3 formalism give a similar structure of the wall heat fluxes as WBCK-RMF3, but that the values are under-predicted by a significant factor. So once again it seems that even though the RMF3 is twice as expensive as the WSGG3 and 7 times as expensive as WSGG1 it is the best compromise.

Conclusion

As the gas-radiation coupling is strong in oxyfuel combustion it is crucial with a good handling of the radiation modeling. Furthermore it is extremely important to design the combustion chamber by e.g. introducing diluents such that the walls do not overheat. Using CO_2 as a diluent is an obvious choice since it effectively shields the walls from the radiative heat at the same time as it does not introduce any extra post combustion problems.

Since radiation modeling is very complex one can not solve the exact equations, but must rely on approximate models. Which model to chose is often a compromise between accuracy and speed, and we find that the discrete ordinate model with the WBCK method and the restricted multiple gases formalism with 3 absorption bins (RMF3) is a good compromise for oxyfuel combustion.

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References

[1] A. Beltrame, P. Porshnev, W. Merchan-Merchan, A. Saveliev, A. Fridman, L. A. Kennedy, O. Petrova, S. Zhdanok, F. Amouri, and O. Charon. Soot and no formation in methane-oxygen enriched diffusion flames. *Combustion & Flame*, 124:295–310, 2001.

[2] T. F. Smith, Z. F. Shen, and J. N. Friedman. Evaluation of coefficients for the weighted sum of gray gas model. *Journal of Heat Transfer*, 104:602–608, 1982.

[3] M. K. Denison and W. A. Fiveland. A correlation for the reordered wave number of the wide band absorptance of radiating gases. *Journal of Heat Transfer*, 119:853–856, 1997.

[4] J. Ströhle. *Spectral modeling of radiative heat transfer in industrial furnaces.* Dr. ing. thesis, University of Stuttgart, Stuttgart, October 2003. ISBN 3-8322-2492-0.

[5] I. R. Gran. *Mathematical modeling and numerical simulation of chemical kinetics in turbulent combustion.* Dr. ing. thesis, University of Trondheim, Norwegian Institute of Technology, Division of Thermodynamics, Trondheim, May 1994. ISBN 82-7119-651-0.