An alternative method to optimise the SLW Grey Gases

2012 J. Phys.: Conf. Ser. 395 012007

(http://iopscience.iop.org/1742-6596/395/1/012007)

An alternative method to optimise the SLW Grey Gases.

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Abstract. The industrial combustion sector needs relatively simple but accurate radiation gas model to perform multiphysics simulations. Built with high resolution spectral absorption line databases, the Spectral-Line-Weighted-Sum of Grey-Gases model (SLWSGG) with a restricted number of grey gases, may meet this need. This paper presents an easier method to optimise the SLW grey gases in comparison with the original method. The optimisation procedure proposed in this work is based on total quantities values (radiative fluxes or source terms) analytically calculated on the equivalent 1D medium.

Nomenclature			
Cabs	absorption cross-section, $mol.m^{-2}$	x	Cartesian coordinate
F	radiation heat flux, $W.m^{-2}$	Y	mole fraction
I	radiation intensity, $W.m^{-2}$	*Greek symbols*	
k	absorption coefficient, m^{-1}	ε	total emissivity
L	path length, m	η	wave number, m^{-1}
M	number of path lengths	ω_i	weight factor for grey gas j
N_s	molar density, $mole.m^{-3}$	ω_0	weight factor for clear gas
P	total pressure	*Subscripts*	
Q	radiation heat flux divergence, $W.m^{-3}$	loc	local value
s	directional path, m	ref	reference value
T	temperature, K		

1. Background

There is still a need in the industrial combustion sector for an easy-to-use, not too time-consuming and nevertheless reasonably accurate radiative model for high temperature gases. As the absorption coefficient of combustion gases strongly varies with temperature, wavelength, composition and pressure, these criteria are hard to meet.

Commercial codes often rely on rather simple absorption models for gases to solve the Radiative Transfer Equation (RTE) in multiphysics simulations. The relatively simple Weighted-Sum-of-Grey-Gases model (WSGG) has been first developed by Hottel and Sarofim [1] and is still widely used in the industry. It uses emissivity values to determine the grey gas absorption coefficients and the associated weights. The radiative heat transfer rate can then be calculated for each grey gas *(1)* or with a global absorption coefficient. Such a model, formulated in terms of absorption coefficient, allows any solution method for the radiative transfer equation.

$$\frac{dI_j}{ds} = -k_j \cdot I_j + \omega_j \cdot k_j \cdot I_b \qquad I = \sum_{j=1}^{n+1} I_j \tag{1}$$

2. The Spectral-Line WSGG model

In the SLWSGG of Denison &Webb [2, 3, 4, 5, 8], Absorption Line Blackbody Distribution Functions (ALBDF) are built using high resolution spectral absorption coefficient databases. ALBDF are used to calculate the model grey gases parameters (ω_j, k_j). The accuracy of the model depends on the number of GG and on the method used to determine the local grey gases parameters needed when solving the RTE. It is not desirable to optimise the grey gases for each local condition (T_{loc}, Y_{loc}) in the gaseous domain. Therefore, the optimisation procedure considers the mean thermophysical state of the medium to calculate de reference grey gases parameters. The local grey gases parameters are then obtained from these reference values by means of assumptions: this is the reference approach. Using the reference approach to deduce the local parameters speeds up the computations but generates errors because the assumptions simplify the behaviour of the gases absorption spectra.

In the original SLWSGG model, the optimisation process is based on total emissivity values calculated for a series of path lengths (L) covering the domain of interest. This choice is not obvious in complex multidimensional systems nor even in 1D problems. The optimisation results depend on the number and the values of the chosen path lengths. We have then tried other optimisation methods that leave less degree of freedom.

Derived from Denison & Webb's SLWSGG, Solovjov et al [6] developed the **SLW-1** method which only uses 1 optimised grey gas (and one clear gas) but, as accuracy generally improves as the number of grey gases increases, we investigated a 3 grey gases optimisation procedure in order to obtain a good balance between precision and computational time.

3. The SLWs and their grey gas(es) optimisation processes

The SLWs models use ALBDF functions [5] which are expressed in terms of absorption cross section: $Cabs=k.N_s$. With the reference approach, a single absorption spectrum is assumed to be representative of the entire gaseous domain. A single temperature and a single molar concentration are therefore chosen in order to characterise the domain. The objective of the optimisation process is, for reference conditions (T_{ref}, Y_{ref}, P_{atm}), to replace the complex absorption coefficient spectrum of the real absorbing species (*fig.1*) by 1 (SLW-1) or 3 (SLW-3) optimised grey fictitious gases (=> 1 or 3 Cabs values). A part of the absorption cross section spectrum is allocated to each grey gas. The weight of a grey gas is calculated with the ALDF considering the 2 Cabs values that border its partition (*fig.1*). The weight of the clear gas is obtained with *(2)*:

$$\omega_0 = 1 - \sum_{j=1}^{1or3} \omega_j \qquad (2)$$

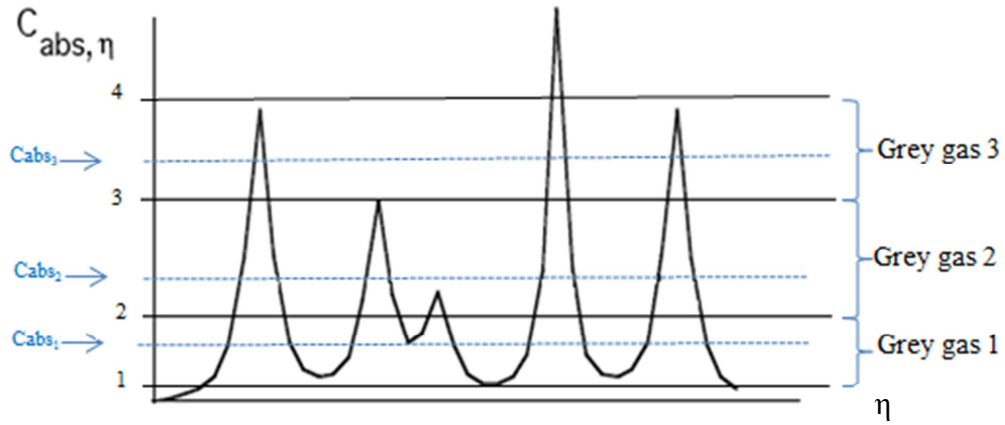

Figure 1: the absorption cross-section spectrum and the 3 fictitious grey gas partitions

When solving the RTE, the reference approach calculates local values (ω_{loc}, k_{loc}) from the reference parameters (with no more optimisation) by using assumptions. In the Denison & Webb's model, the reference grey gases parameters are optimised by minimising (least-squares minimisation) the relative

errors between the total emissivity values calculated with 3 optimised GG and the true emissivities (computed using 20 GG) for a set of M path lengths (L) covering the domain of interest *(3)(4)*. So the range, the number of values and the repartition of the path lengths within the range have to be chosen. The combinations are numerous and the results of the optimisation, as well as the solution of the RTE, depend on these choices.

$$\text{to minimise}: \sum_{i=1}^{M}\left(1-\frac{\varepsilon_{3GG\,Li}}{\varepsilon_{20GG\,Li}}\right)^2 \qquad \varepsilon_{3GG\,Li}=\sum_{j=1}^{3}\omega j\cdot\left(1-e^{-k\,j\cdot Li}\right) \qquad (3)\ (4)$$

Our aim was to tune a systematic and robust procedure for optimising the grey gases. We have tried different combinations but none was the best for all the 1D cases tested. The optimisation was tricky: different initial values lead to different solutions because the function to minimise had local minima. The reference (average) temperature can be understood, and consequently calculated, in different ways. We noticed that the results were generally better using the T^4 field instead of T field.

In the SLW-1 model of Solovjov et al. [6], a reference state is also needed. An isothermal-homogeneous gaseous layer bounded by black walls at 0K is used to fit the SLW-1 reference parameters: k_{1ref}, ω_{1ref}. These parameters are determined with a constraint related to 1D exact total quantities (F, Q…). Those have to be correctly replicated by the SLW-1 model at two different locations (optimised positions) in the domain. The reference cross-sections are calculated and the local parameters (k_{1loc}, ω_{1loc}) are then estimated using the original SLW reference approach. Solovjov et al. showed that using F and Q values gave rather good results. , The present work derives from their developments.

4. The modified optimisation procedure

In this work, the Solovjov approach is applied to develop SLW-3 optimisation methods. An average thermophysical state is used in the optimisation process. The reference temperature is calculated using the T^4 field and the reference molar fraction is the spatial average value.

Considering 25 spatial locations on the reference equivalent model (isothermal, homogeneous between 2 black cold walls), 25 flux or source term values are calculated analytically. The true (F or Q) values are calculated with 20 GG. This corresponds to 41 Cabs logarithmically spaced. The 3GG's parameters (i.e. 7 Cabs see fig.1) are then optimised by minimising the relative errors that result when F (or Q) values are calculated with only 3GG (least-squares method). Flux and source term present symmetrical profiles on the reference equivalent model. The 25 locations are therefore taken over half of the domain.

5. Results

The method is tested on 1-D problems at atmospheric pressure. In these problems water vapour or carbon dioxide (in air) between two infinite parallel walls is considered. The source term profiles of these gaseous media are calculated using the Discrete Ordinates Method (S20). The results obtained are compared with LBL, 3 optimised grey gases (based on emissivity values) and 20 grey gases calculations.

For the 3 GG optimisation based on emissivity, we took path lengths ranging from D/100 to 10D and used 5 path lengths by decade.

The first two test cases come from Denison's dissertation [5] and have been used in the SLW-1 publication [6].

5.1. Water vapour: isothermal, homogeneous

In this test case, water vapour at 1500K, Y=0.5 between 2 grey walls (ε=0.6) at 1200K and 600K is considered.

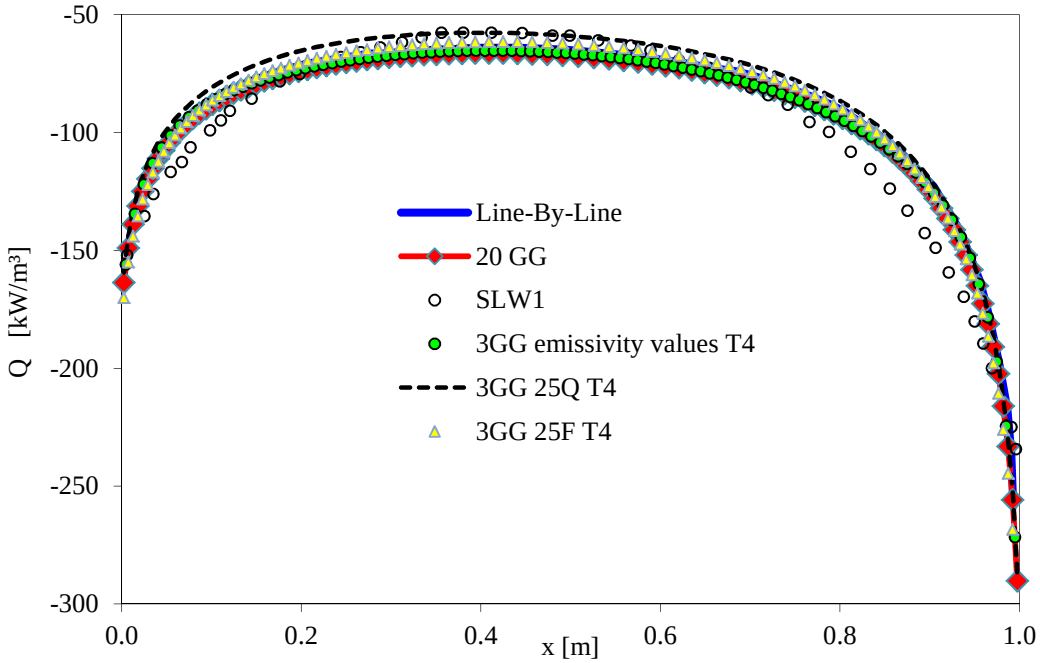

Figure 2: source term profiles for 50% H_2O at 1500K

The line-by-line profile comes from Denison's work [5], the SLW-1 profile comes from [6] and uses an optimisation procedure based on 2 Q values, the other profiles have been calculated with 20 GG or 3 optimised GG.

We have tested the new method of optimisation with 25 locations for flux (F) and source terms (Q) values.

Except the SLW-1 profile and the profile obtained with the 25 Q values, all the other profiles are very close to each other.

5.2. Water vapour: isothermal, non-homogeneous

This second problem is relative to water vapour 10% in air between 2 black walls at 1250K and 750K. The walls are 2 m distant (D). The gas has a cosinusoidal temperature profile (*fig.3*):

$$T(x) = 1000 + (500/2)\cos(\pi x/D)$$

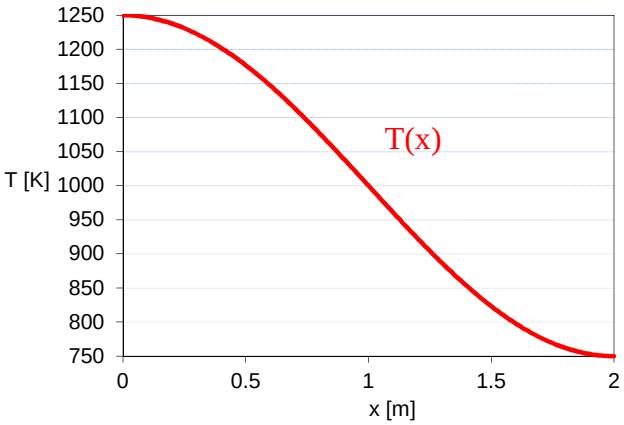

Figure 3: temperature profile of case test 2

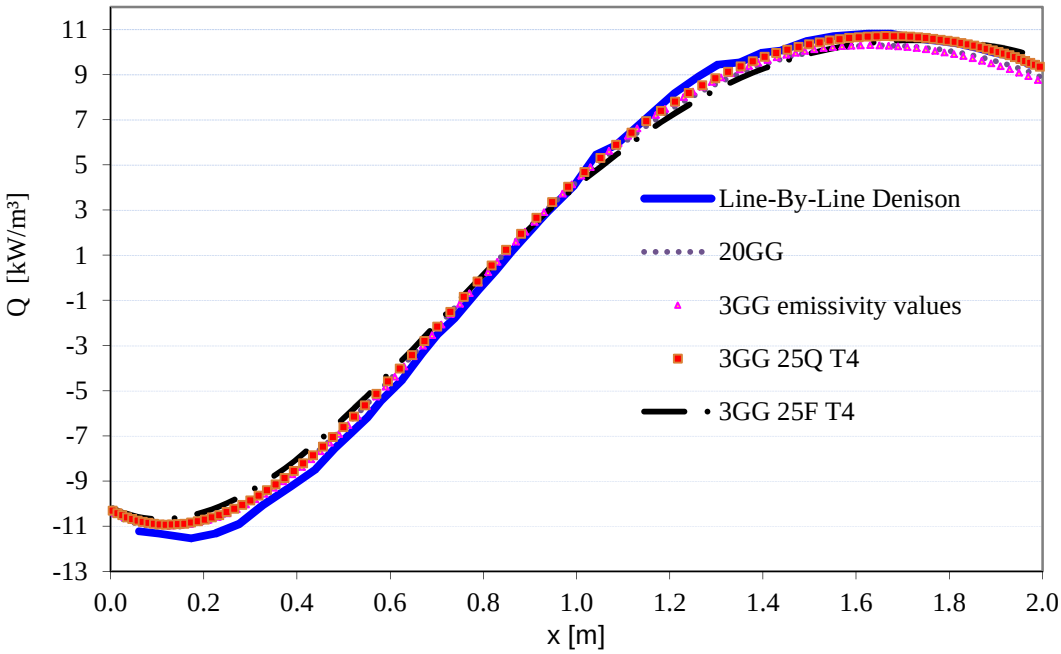

Figure 4: source term profiles for 10% H_2O with cosinusoidal temperature profile

The figure 4 also presents source term profiles very close to each other. The profile obtained by the SLW-1 model is very close to the Line-by-line profile (it is not represented here for readability reason).
The optimisation procedure that uses source term values (3GG 25Q T4) seems to be slightly better in the cold part of the domain than those obtained with fluxes values. The optimisation procedure based on emissivity values (3GG emissivity values) gives a very good profile.

5.3. Carbon dioxide : non- isothermal, non-homogeneous
The third case is taken from the work of Weçel et al [7]. They use a more recent spectral database (CDSD 1000-2003). It is interesting to see if the D&W's correlation, built with an older database (HITRAN 1991 D&W [5]), would give very different results.
The figure 6 presents the evolution of the directional intensity emitted by a black wall at 800K which propagates through a participating gaseous medium.

Sinusoidal profiles of concentration and temperature are considered over 1 meter (D):

$$T(x) = 800 + (1500-800)\sin(\pi x/D)$$
$$Yco_2(x) = 0.1 + (0.01 - 0.1)\sin(\pi x/D)$$

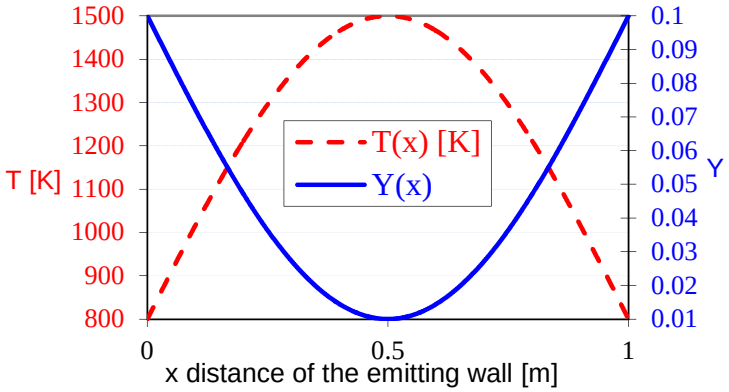

Figure 5: temperature and molar fraction profiles for the third test case

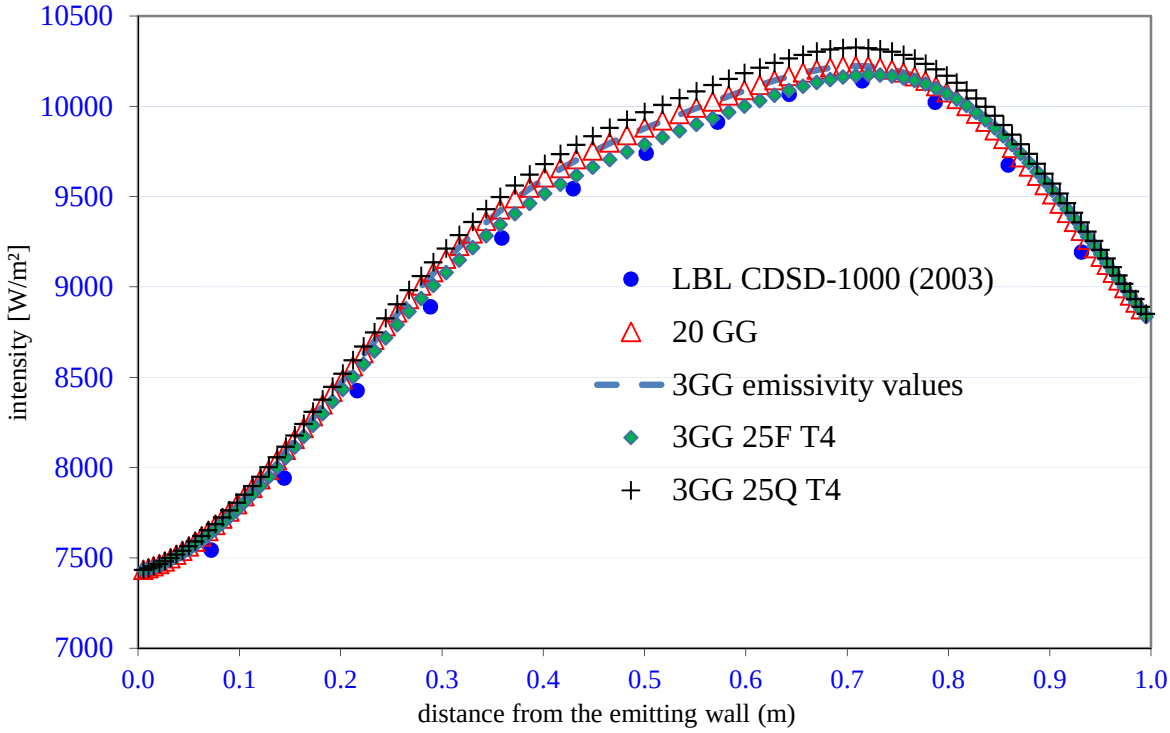

Figure 6: directional intensity profiles for CO_2 with sinusoidal temperature and concentration variations

The 3GG optimised with emissivity values gives excellent results as the 3GG optimized with F Values. For x values over 0.6 m, the profile calculated with 3GG optimised with F values is slightly less distant from the 20GG profile than the one calculated with 3GG optimised with Q values. For this test case, the older database does not seem to give very different results from the ones obtained by LBL calculations with the CDSD-1000 database.

6. Conclusion

The alternative optimisation procedure proposed in this work provides a more straightforward method to optimise the SLW's grey gases. The results obtained are rather good. The original optimisation procedure, that uses emissivity values, can give better results but the choice of the path lengths distribution is not obvious and none of those we tested proved to be the best for all cases considered [6]. With this new procedure there is no need to tune parameters.

The procedure could be extended to 2-D and 3-D radiation problems using a reference 1-D model defined as an isothermal and homogeneous medium between 2 black walls at 0K. The distance between the walls would be then related to the mean beam length of the 2D or 3D problem.

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