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Validity limits for the global model FS-SNBcK for combustion applications

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Abstract
In this work the Full Spectrum based on the Statistical Narrow Band with the correlated k approximation (FS-SNBcK) is presented. The idea behind the model is to group the narrow bands using the Malkmus model, in order to build a Full Spectrum representation of the space of frequencies. All narrow bands are grouped and weighted by the Planck function to take into account the variation of the blackbody intensity over the whole spectrum. In this paper, validity limits of the model are studied, using a one dimensional isothermal homogeneous gas layer. The influence of species concentration, layer thickness and temperature are tested. An detailed mathematical formulation of the model is presented. Finally, 3D simulations were performed to check the efficiency of the model against other spectral methods.

1. Introduction

Only recently Large Eddy Simulations (LES) have been coupled with detailed radiation [15, 5]: CPU time is still a main issue for non-stationary flames. To solve the Radiative Transfer Equation (RTE) on combustion application the Discrete Ordinates Method is chosen, because it offers the best compromise between CPU time and accuracy [7, 8] and could be used to calculate complex geometries. This method relies on the 4π solid angle discretization using angular quadrature sets (directions and weights).

For spectral properties, a k-formulation (where k is the absorption coefficient) is required to be compatible with the differential form of the RTE. An exact description of spectral properties needs a line by line (LBL) model, but these models have the disadvantage of having a high computational cost.

The SNBcK model uses a narrow band approach and offers a good quality radiation/LES simulations. But this model can not be afforded in coupled situations because it is still too expensive. This model solves the RTE at least 5 times (5 quadrature points) per band. Typically 367 narrow bands are used. These represents a total of 5x367 = 1835 resolutions of the RTE performed for one given direction.

A good alternative to this SNBcK is the use of a global model such as the well known Weighted Sum of Gray Gases (WSGG)[6]. It is fast but no accurate enough when the studied situation is far from the one used to fit it. Various authors have already proposed the use of these global models. Denison and Webb [2, 3] developed the spectral-line-based

weighted-sum-of-gray-gases (SLW) model, in which line-by-line databases are used to obtain weight factors for the WSGG model. The Absorption Distribution Function have some similarities with the SLW and was developed by Riviere et al. [14, 13]. Modest and Zhang wrote a mathematical formulation that allows to write the k-distribution for the whole spectrum [12].

Another approach in the frame of the SNB models, was proposed by Liu et al.[9], they proposed a method which provides a good accuracy by reducing the number of resolutions of the RTE. By using a band lumping strategy, authors have shown that a maximum of 10 narrow bands could be grouped without loosing accuracy. The SNBcK model is based on the narrow band approximation, in which the Planck function is considered constant on a narrow band. The band lumping strategy is limited by this approximation. In a publication Liu et al. [11] proposed to group all bands to build the full spectrum statistical narrow band ck based (FS-SNBcK). In this model all bands are grouped and weighted using the Planck function to take into account the variation of the blackbody function over the whole spectrum.

The aim of the present work is to present a detailed mathematical formulation then to study the limits of validity of this model. To the authors knowledge, it is the first time that the mathematical formulation of the probability density function and the cumulative are used to describe the FS-SNBcK model.

2. Formulation and definition of the FS-SNBcK model

2.1. Integration over the spectrum

Lets define F, a function of the absorption coefficient κ_ν and the integral I over a narrow band $\Delta\nu$ as:

$$\overline{I_{\Delta\nu}} = \int_{\Delta\nu} L_{b,\nu} F(\kappa_\nu) d\nu \tag{1}$$

Where $L_{b,\nu}$ is the Planck function depending on the temperature and the frequency. If the interval $\Delta\nu$ is not too large the Planck function can be considered constant over the narrow band and equal to $\overline{L_{b,\Delta\nu}}$:

$$\overline{I_{\Delta\nu}} \approx \overline{L_{b,\Delta\nu}} \int_{\Delta\nu} F(\kappa_\nu) d\nu = \overline{L_{b,\Delta\nu}} \Delta\nu \overline{F_{\Delta\nu}} \tag{2}$$

In order to avoid a line-by-line description of the spectrum, Domoto [4] has introduced the function f, which is the probability density function of κ aside the frequencies, representing the k-distribution in the narrow band:

$$\overline{F}_{\Delta\nu} = \frac{1}{\Delta\nu} \int_{\Delta\nu} F(\kappa_\nu) d\nu = \int_0^\infty F(\kappa) f(\kappa) d\kappa \tag{3}$$

The mean value of F can be obtained by a discrete integration over all narrow bands:

$$I_{tot} = \sum_{i=1}^{N_B} \overline{I_{\Delta\nu_i}} \Delta\nu_i = \sum_{i=1}^{N_B} \Delta\nu_i \overline{L_{b,\Delta\nu_i}} \int_0^\infty F(\kappa) f_i(\kappa) d\kappa \tag{4}$$

where subscript i denotes the band number, N_B the total number of bands and $f_i(\kappa)$ is the PDF on the i^{th} band. Variables ν_i and κ are independent so the discrete integration on i and the integration on ν can be switched, leading to:

$$I_{tot} = \int_0^\infty \left(\sum_{i=1}^{N_B} \Delta\nu_i \overline{L_{b,\Delta\nu_i}} F(\kappa) f_i(\kappa) \right) d\kappa \tag{5}$$

This expression may be rewritten as the *expectancy* of the function $F(\kappa)$, if the corresponding probability density function is correctly defined. By definition the PDF must be normalized such as:

$$\int_0^\infty \sum_{i=1}^{N_B} \Delta\nu_i \overline{L_{b,\Delta\nu_i}} f_i(\kappa) d\kappa = \sum_{i=1}^{N_B} \Delta\nu_i \overline{L_{b,\Delta\nu_i}} \times \underbrace{\int_0^\infty f_i(\kappa) d\kappa}_{\text{= 1, by definition}} = \frac{\sigma T^4}{\pi} \tag{6}$$

So the integration over the spectrum may be rewritten as:

$$I_{tot} = \frac{\sigma T^4}{\pi} \int_0^\infty \underbrace{\sum_{i=1}^{N_B} \frac{\Delta\nu_i \overline{L_{b,\Delta\nu_i}} f_i(\kappa)}{\sigma T^4/\pi}}_{f_{FS}(\kappa)} F(\kappa) d\kappa \tag{7}$$

Where f_{FS} represents the *full spectrum normalized probability density function*.

2.2. Introduction of the ck approximation in the FS-SNBcK model

The Malkmus model allows to get an analytical expression for the mean transmissivity $\overline{T}_{\Delta\nu}$ with some properties of the spectrum according to specific assumptions.

$$\overline{T}_{\Delta\nu}(l) = \exp\left[\Phi_{\Delta\nu} \left(1 - \left(1 + \frac{2\overline{\kappa} l}{\Phi_{\Delta\nu}} \right)^{1/2} \right) \right] \tag{8}$$

where $\overline{\kappa}$ is the average value of the absorption coefficient over the narrow band, and $\Phi_{\Delta\nu}$ is the shape parameter. Data for $(\overline{\kappa}, \Phi_{\Delta\nu})$ were taken from the SNB parameters database of Taine and Soufiani [17], for temperatures between 300K and 2900K and for 367 bands of width $\Delta\nu = 25$ cm^{-1}.

Using eq.(3), the mean transmissivity over a narrow band is given by:

$$\overline{T}_{\Delta\nu}(l) = \int_0^\infty \exp(-\kappa l) f(\kappa) d\kappa \tag{9}$$

Domoto [4] has shown that $f(\kappa)$ is the inverse Laplace transform of the mean transmissivity, given by the Malkmus model. The function $f(\kappa)$ is not monotonous and it is more convenient to introduce the cumulative function $g_i(\kappa)$, over the i^{th} narrow band:

$$g_i(\kappa) = \int_0^{\kappa} f_i(\kappa')d\kappa' \tag{10}$$

$g(\kappa)$ is a monotonously increasing function in the interval $[0;1]$ which allows to inverse it to get the function $\kappa(g)$. The inverse function $\kappa(g)$ can thus be defined. If the shape of the spectrum is not modified by the pressure and the temperature along an optical path, the ck-approximation is achieved. Using the Malkmus model for the transmissivity Domoto has shown that the function $f(\kappa)$ is an Inverse Gaussian distribution, $g(\kappa)$ uses erfc functions [4]. This function is inverted numerically.

Using the cumulative function $g(\kappa)$, eq.(3) could be written as:

$$\overline{F}_{\Delta\nu} = \int_0^1 F(\kappa(g))dg \tag{11}$$

The *full spectrum cumulative function* $g_{FS}(\kappa)$ is defined as:

$$\begin{aligned} g_{FS}(\kappa) &= \int_0^{\kappa} f_{FS}(\kappa')d\kappa' = \int_0^{\kappa} \sum_{i=1}^{N_B} \frac{\Delta\nu_i \overline{L_{b,\Delta\nu_i}} f_i(\kappa')}{\sigma T^4/\pi} d\kappa' \\ &= \sum_{i=1}^{N_B} \frac{\Delta\nu_i \overline{L_{b,\Delta\nu_i}}}{\sigma T^4/\pi} \underbrace{\int_0^{\kappa} f_i(\kappa')d\kappa'}_{g_i(\kappa)} \end{aligned} \tag{12}$$

From eq.(12) it can be noticed that g_{FS} is monotonically increasing with κ, like each function $g_i(\kappa)$ does, and can also be inverted numerically to obtain $\kappa(g_{FS})$, eq.(6) then becomes:

$$I_{tot} = \frac{\sigma T^4}{\pi} \int_0^1 F(\kappa(g_{FS}))dg_{FS} \tag{13}$$

As the cumulative function is monotonically increasing, the numerical resolution of the integration could be achieved either with a statistical method or using a Gauss quadrature. If a quadrature is used over N_q points, eq.(13) can be written:

$$I_{tot} \approx \frac{\sigma T^4}{\pi} \sum_{j=1}^{N_q} w_j F(\kappa(g_{FS,j})) \tag{14}$$

It is only at this last step that the calculation of I_{tot} (over the entire spectrum) is approximated numerically, using a pseudo-spectral quadrature.

2.3. Radiative properties of the mixture Modeling

To take into account multicomponent mixtures several models are proposed by Liu [10]. The model based on the optically thin limit provide $\langle \kappa_{mix} \rangle$ and $\Phi_{\Delta\nu,mix}$ for a mixture of N_g species, of parameters $\overline{\kappa}_n$ and $\Phi_{\Delta\nu,n}$:

$$\langle \kappa_{mix} \rangle_{\Delta\nu} = \sum_{n=1}^{N_g} \overline{\kappa}_n \qquad \text{and} \qquad \frac{\langle \kappa_{mix} \rangle_{\Delta\nu}^2}{\Phi_{\Delta\nu,mix}} = \sum_{n=1}^{N_{gas}} \frac{\overline{\kappa_n}^2}{\Phi_{\Delta\nu,n}} \tag{15}$$

where $\overline{\kappa}_n$ is the average value of the absorption coefficient over the narrow band, and $\Phi_{\Delta\nu,n}$ is the shape parameter for the n^{th} gas. The main advantage of this model is to insure a good compromise between accuracy and CPU time.

3. Absorption of a one dimensional gas layer

To separate spectral aspects from geometrical aspects and test the FS-SNBcK model, the absorption of a one dimensional isothermal homogeneous gas layer is considered. Gases containing one or more of the following species were studied: H_2O, CO_2, CO. The FS-SNBcK model is compared to the Malkmus model, which represents the reference model for the one dimensional study.

In this configuration the mean intensity of the narrow band absorbed by the gas layer is:

$$\overline{I}_{\Delta\nu}(l) = \int_{\Delta\nu} \exp(-\kappa_\nu l) L_{b,\nu} d\nu \tag{16}$$

The total intensity absorbed by the spectrum in the FS-SNBcK is given using eq.(13) with $F(\kappa_\nu) = T(l) = \exp(-\kappa_\nu l)$ and calculated using a Gauss Legendre quadrature according to eq.(14).

3.1. Influence of the mixture composition

The absorption is calculated on an homogeneous and isothermal gas layer containing only one species at different temperatures, with gas column length of $l = 1m$. *Figure 1* shows that in the case of pure H_2O, the FS-SNBcK calculation with $N_q = 5$ gives an error of about 10%. Nevertheless, when the number of quadrature is augmented to $N_q = 10$ a very good agreement with the Malkmus model is obtained. In the pure CO case, the error with $N_q = 5$ reaches a value of nearly 100%. For both pure CO_2 and CO cases, a higher N_q is needed to fit with the Malkmus case, typically $N_q = 30$.

Figure 2 shows the cumulative functions, g_{FS} for different gases. As CO_2 and CO do not emit in all bands contrary to H_2O (96 bands for CO_2, 48 bands for CO) some values of κ are close to zero and the cumulative function is non zero only in a small part of the interval [0;1]. More quadrature points are needed to resolve the spectrum. It is also noticed that for high temperatures the gradient of the cumulative function is higher.

Theoretically by increasing N_q to infinity, the $\kappa(g)$ should always be well resolved.

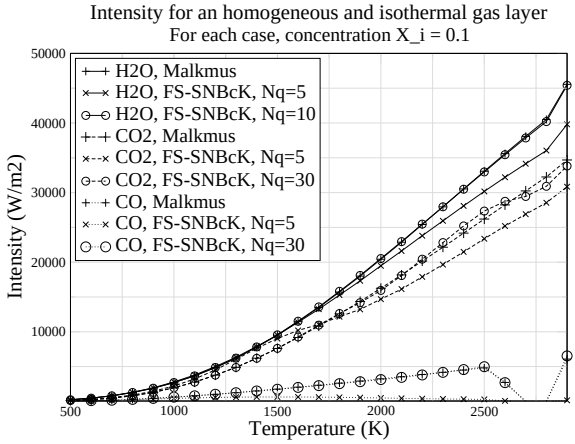

Fig. 1 — Influence of N_q for a single species at different temperatures

However if the gradient of the function is too strong, the numerical inversion of $g(\kappa)$ fails. An example with a high temperature and 20% molar fraction of CO gives an error of 30% even with $N_q = 30$. For cases containing high concentrations of CO this model must be the used with care, in particular if the temperature is high.

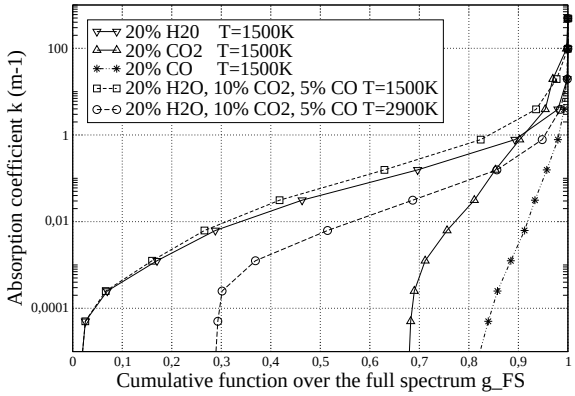

Fig. 2 — Cumulative function for different gas mixtures at 1500 and 2900K

3.2. Influence of the gas optical thickness

In a second step the influence of the gas optical thickness is investigated. In this case the gas layer is composed of 20% H_2O, 10% CO_2, 5% CO molar fraction. The absorption of the gas layer is calculated at several temperatures for three thicknesses: $l = 0.1m$, $l = 1m$ and $l = 10m$ an plotted in *figure 3*.

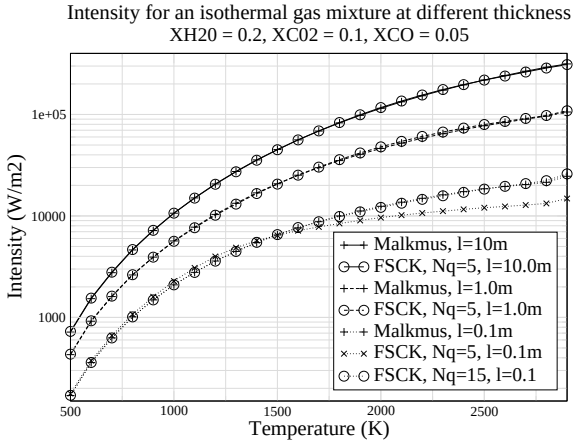

Fig. 3 — Influence of the gas thickness for a mixture of gases at different temperatures

Figure 3 shows that a high number of quadrature points are needed to fit with the reference when the gas layer is thin. To explain this behavior, the relative error on the transmissivity, $T(l) = \exp(-\kappa l)$, is analyzed:

$$\frac{\Delta T}{T} \sim \frac{\exp(-\kappa l)\kappa l}{1-\exp(-\kappa l)} \frac{\Delta \kappa}{\kappa} \tag{17}$$

In this expression when l increases, the relative error tends to zero. For the optically thin limit when l tends to 0, $\frac{\Delta T}{T} \approx \frac{\Delta \kappa}{\kappa}$, and the calculation of the absorption is more sensitive to the error on κ. For the thick case even if the relative error is smaller, the model will is limited by the mixture modeling (cf. section 2.3.) and the ck-approximation.

4. 3D Calculations

To validate geometry influence of the FS-SNBcK model, 3D calculations are performed using a DOM code (*DOMASIUM*[1]). Two benchmark cases are tested [1] using an S4 angular quadrature: a homogeneous cylinder and an an-isothermal and non-homogeneous cylinder.

These two radiative heat transfer problems are in two-dimensional axisymmetric enclosures with black walls. Atmospheric pressure is considered in all cases. In both tests calculations are compared to available reference solutions (a ray-tracing solution or a Monte-Carlo Method all together with k-distribution). Tests include comparisons with the SNBcK model (reference solution) and the WSGG model (faster model). The WSGG model parameters are given in [16].

The first case is a cylindrical enclosure of length $L = 3.0m$, a radius $R = 0.5m$ and was resolved using a mesh with 19343 tetrahedron cells. The temperature of the walls is $300K$. Species molar fractions of the gas are 20% H_2O, 10% CO_2 and 70% N_2. There

[1] http://www.cerfacs.fr/domasium

is no soot and the temperature of the medium is $1800K$.

The second case is a cylinder of length $L = 1.2m$, a radius $R = 0.3m$ and was resolved using a mesh with 27749 tetrahedron cells. The walls are black at $800K$, except the right wall ($x = L$), which is maintained at $300K$. The temperature and the molar fractions of H_2O and CO_2 are given by analytical profiles:

$$\begin{aligned} T(x,r) &= 800 + 1200 * (1 - r/R)(x/L) \\ X_{H_2O} &= 0.05\left[1 - 2(x/L - 0.5)^2\right](2 - r/R) \\ X_{CO_2} &= 0.04\left[1 - 3(x/L - 0.5)^2\right](2.5 - r/R) \end{aligned} \tag{18}$$

The soot volumetric fraction is $f_v = X_{SOOT} = 10^{-7}$. Spectral absorption coefficient for soot is calculated as $\kappa_{\nu,soot} = 5.5 f_v \nu$.

Figure 4 and *figure 5* show that the calculation of the radiative source term S_r, using the FS-SNBcK, gives results in very good agreement with the SNBcK model. For the two test cases only five quadrature points are needed to obtain a good accuracy. It is also shown that this model is clearly more accurate than the WSGG model due to the fact that the global data of the mixture is modeled from the SNB database. It is noticed that for case 2 the WSGG model gives better results than in case 1 because the presence of soot yield the medium more gray.

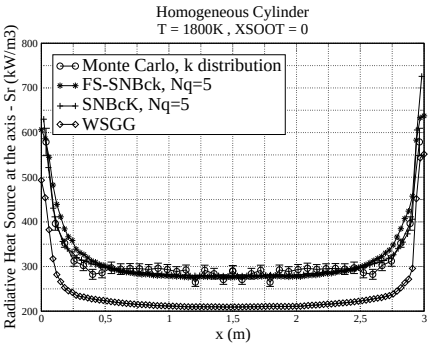

Fig. 4 — Case 1: radiative source term S_r along the central axis for the homogeneous cylinder. The reference solution is a Monte-Carlo solution [1]

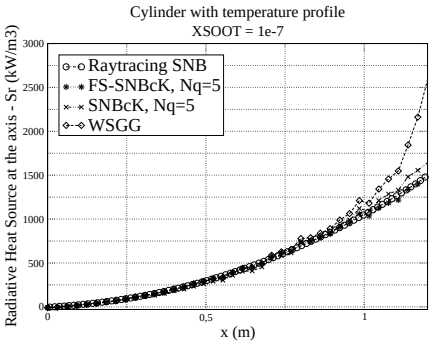

Fig. 5 — Case 2: radiative source term along the cylinder axis for the different spectral models. The reference solution is a ray-tracing solution [1]

5. Calculation time cost

Table 1 shows that in the one dimensional calculation, where the time calculation is devoted mostly to the spectral calculation, the FS-SNBcK is not faster than the SNBcK model: the same number of calculations are performed in the two models. To calculate $g_{FS}(\kappa)$ in eq.(12) a loop over all bands is done. Then eq.(14) requires an iterative time

Tab. 1 — *Time calculation for the FS-SNBcK in 1D and 3D calculation*

	Test 1D N_q=5	Test 1D $N_q = 10$	Test 1D $N_q = 20$	Test 3D Case 1	Test 3D Case 2
SNBcK	9.0 ms	17.2 ms	37.2 ms	40 m36.2 s	67 m49.5 s
FS-SNBcK	24.7 ms	46.0 ms	100.0 ms	0 m8.1 s	8 m51.6 s
WSGG	–	–	–	0 m6.6 s	0 m10.2 s

consuming process to inverse numerically $g_{FS}(\kappa)$. The inversion is longer to achieve for FS-SNBcK because the gradient of function $g_{FS}(\kappa)$ is higher (less than 10 iterations for SNBcK, between 20 to 30 iterations for FS-SNBcK).

The advantage of a global model as FS-SNBcK for 3D calculations is clearly demonstrated by the time efficiency on *table 1*. The number of resolutions of the RTE is strongly reduced. In case 1, homogeneous case, only one absorption coefficient is calculated over the domain. The time calculation of FS-SNBcK is about 300 time shorter than the SNBcK, very close to the number of narrow bands (367). For case 2, non-homogeneous case, the calculation time is reduced by one order of magnitude compared to SNBcK case. In this case spectral calculations account for 97% of the total calculation with the FS-SNBcK model. This shows that most of the effort should be made in the improvement of the spectral calculation for this model.

6. Conclusions

The full spectrum based on the statistical narrow bands model with the ck-approximation was studied in order to validate its implementation on combustion applications. An detailed mathematical formulation of the model has been proposed. Then the limits of validity of the model were investigated in the case of a one dimensional gay layer.

It was shown that the model fits well with the Malkmus model if enough quadrature points are used. For gases with a high concentration of CO, which does not emit in all bands, the calculation differs from the reference value at high temperature. In the optically thin case, more quadrature points are needed to calculate accurately the absorption.

In 3D calculations the model gives very good results even with only five quadrature points. The calculation times are substantially reduced because the number of resolutions of the RTE is reduced from 1835 to 5.

The next objective is to improve the time calculation using a tabulation technique for the spectral properties of the FS-SNBcK model. This will allow to reduce the calculation time dedicated to spectral calculation and will permit to reach a calculation time comparable with those obtained with the WSGG model.

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