Modelling turbulence-radiation interactions for large sooting turbulent flames

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1. Motivation and objectives

Large-scale turbulent flames and fires are strongly influenced by radiative energy transport. Especially in fires, fluid dynamics are governed by buoyancy, and hence, by the density and temperature distribution (Joulain (1998); Drysdale (1999); Tieszen (2001)). In pool fires, also the fuel mass flow rate is determined through radiative energy transfer from the flame to the liquid fuel, which thereby determines the evaporation rate. An accurate description of radiative energy transfer, which, in fires, is mainly caused by soot radiation, is therefore mandatory in numerical simulations.

Since a detailed description of radiation using, for instance, a discrete ordinate method is usually very expensive in numerical simulations, radiation is most commonly described using simplified models, such as the Milne-Eddington diffusion equations, valid in the limit of isotropic radiation, the Rosseland model, valid for high opacity media, or the optically thin model, valid for non absorbing media. Another simplification that is often made is neglecting turbulence-radiation interactions (TRI), although these have been found to be important, for instance, in pool fires (Tieszen (2001)). The aim of this paper is to provide a closed averaged radiation model accounting for TRI, which is simple and cost effective enough to be applied in numerical simulations.

A macroscopic radiation model, the M_1-model, which has also been called the maximum entropy closure radiation model, has been developed successively by Minerbo (1978), Levermore (1984), Anile *et al.* (1991), Muller & Ruggeri (1993), Fort (1997), Dubroca & Feugeas (1999), and Brunner & Holloway (2001). This model provides field equations for the radiative energy and the radiative flux vector. The major advantage of this model is that it remains valid independently of the opacity. Ripoll (2002) has developed an averaged form of the M_1-model for turbulent flows. The resulting formulation, however, is very complex and expensive to solve. In the present paper, we develop a simplified formulation of this model, which is better suited for combustion problems, and particularly for fire simulations. It will be shown how various levels of simplified models can be obtained from the M_1-model with mean absorption coefficients (Ripoll *et al.* (2001)), and from these, closed form averaged models will be provided at different approximation levels.

The paper is organized as follows. First, in section 2, we will give a short overview of the M_1 radiation model and define the mean absorption coefficients. In section 3, different approximations will be provided for the mean absorption coefficients and the Eddington tensor, which is the most complex term in the M_1-model. An averaged form of the M_1-model for turbulent flows and closure for various terms will be presented in section 4. The variance of the radiative temperature remains as the only unknown. Finally, in section 5, models of various complexity for this quantity will be provided and discussed.

2. Radiative transfer equations

2.1. *The M_1 radiation model with mean absorption coefficients*

The M_1 radiation model developed by Minerbo (1978), Levermore (1984), Anile *et al.* (1991), Muller & Ruggeri (1993), Fort (1997), Brunner & Holloway (2001), and Dubroca & Feugeas (1999) describes the evolution of the radiative energy E_R and the radiative flux $\vec{F}_R$ of a non-scattering gray medium. Considering a total radiative intensity $I(\vec{r}, t, \vec{\Omega}, \nu)$, where $\vec{r}$ is the position, t the time, $\vec{\Omega}$ the normalized direction vector and nu the frequency, $E_R(\vec{r}, t) = \langle I \rangle_{\Omega,\nu}$ and $\vec{F}_R(\vec{r}, t) = \left\langle \vec{\Omega}\, I \right\rangle_{\Omega,\nu}$ describe the first two moments of the $I(\vec{r}, t, \vec{\Omega}, \nu)$ distribution according to the direction and the frequency. When the medium follows a Rayleigh law, the M_1-model with mean absorption coefficients, developed by Ripoll *et al.* (2001), is written as

$$\partial_t E_R + \vec{\nabla} \cdot \vec{F}_R = c\big[\sigma_P a T^4 - \sigma_E E_R\big] \tag{2.1}$$

$$\frac{1}{c}\partial_t \vec{F}_R + c\ \vec{\nabla} \cdot \left(\vec{\vec{D}}_R\ E_R\right) = -\sigma_F\ \vec{F}_R \tag{2.2}$$

where T is the temperature of the medium, c is the speed of light and the constant a is defined by $a = \frac{8}{15}\frac{\pi^5 k^4}{h^3 c^3} = \frac{4\sigma_{sb}}{c}$. Here, k is the Boltzmann constant, h is the Planck constant, and σ_{sb} is the Stefan-Boltzmann constant.

The mean absorption coefficients, which represent the opacity at the macroscopic level, are denoted by σ_P for the Planck mean absorption coefficient, and σ_E and σ_F for the two effective mean absorption coefficients defined below. The radiative flux is defined by $\vec{F}_R = (F_R^x,\ F_R^y,\ F_R^z)^T$ in $\mathbb{R}^3$. The Eddington tensor $\vec{\vec{D}}_R$ is computed in terms of the Eddington factor $\chi(\|f\|)$ and of the anisotropic factor $\vec{f}$, given by $\vec{f} = (f_x,\ f_y,\ f_z)^T = \vec{F}_R/(cE_R)$ as

$$\vec{\vec{D}}_R = \frac{1-\chi}{2}\ \vec{\vec{\mathrm{Id}}} + \frac{3\chi - 1}{2}\ \vec{n} \otimes \vec{n}, \quad \text{with } \vec{n} = \frac{\vec{f}}{\|f\|}\,. \tag{2.3}$$

Here, $\|g\|$ denotes the Euclidian norm of a vector $\vec{g}$, $\vec{\vec{\mathrm{Id}}}$ is the identity matrix, $\otimes$ stands for the dyadic product, and χ is defined by

$$\chi(\vec{f}) = \frac{3 + 4\|f\|^2}{5 + 2\sqrt{4 - 3\|f\|^2}}\,. \tag{2.4}$$

The radiative pressure is defined from the Eddington tensor as $\vec{\vec{P}}_R = \vec{\vec{D}}_R E_R$ and the radiative temperature is defined through the radiative energy as

$$T_R = \left(\frac{E_R}{a}\right)^{\frac{1}{4}}\,. \tag{2.5}$$

This macroscopic model is hyperbolic and has two equations describing the relaxation towards the radiative equilibrium, which is given by $E_R = aT^4$ and $\vec{F}_R = 0$. Another important property is that the norm of the anisotropic factor $\vec{f}$ is bounded ($\|f\| \in [0, 1]$), which implies that the radiative flux is controlled by the speed of light. At the equilibrium, the anisotropic factor $\|f\|$ is equal to zero, while $\|f\|$ tends to 1 (i.e. $\|F_R\| = cE_R$), when the emission is anisotropic. This corresponds to the transparent limit. This property ensures that the M_1-model stays valid for all values of the opacity, since the speed of light is never exceeded and both opaque and transparent limits are given by the Eddington tensor. The expression for the Eddington tensor D_R, which plays the role of a flux limiter, is derived from an underlying spectral radiative intensity. This intensity can describe a beam (by a Dirac function) as well as an isotropic emission (by a Planck function), and can hence be applied in both the transparent and the opaque limit. Therefore, this model can be applied in fire simulations, where the main difficulty in modeling radiative heat transfer comes from the wide range of opacities of the medium, which leads to anisotropic radiation. This makes the commonly used diffusion models, such as the Milne-Eddington and Rosseland models, and the optically thin model inapplicable.

An interesting alternative formulation of the M_1-model with mean absorption coefficients can be derived by neglecting the time dependent terms in (2.1) and (2.2). Then, a diffusion equation for the radiative energy can be derived by eliminating the radiative flux from these equations as

$$\vec{\nabla} \cdot (\frac{1}{\sigma_F} \vec{\nabla} \cdot (\vec{\vec{D}}_R E_R)) = c\big[\sigma_P a T^4 - \sigma_E E_R\big] \,. \tag{2.6}$$

Similarly, by eliminating the radiative energy, a diffusion equation for the radiative flux is obtained as

$$-\vec{\nabla} \cdot (\frac{\vec{\vec{D}}_R}{\sigma_E} \; \vec{\nabla} \cdot \vec{F_R}) + \sigma_F \vec{F_R} = -c \vec{\nabla} \cdot (\frac{\sigma_P}{\sigma_E} \vec{\vec{D}}_R a T^4) \,. \tag{2.7}$$

Note that taken separately, these equations are unclosed.

2.2. *Definition of the mean absorption coefficients*

For sooting flames, a Rayleigh diffusion law for the spectral absorption coefficient can be employed, and provides the opacity σ as a linear function of the frequency ν as $\sigma(\nu) = C_1 \nu$. The factor C_1 depends then on the soot volume fraction C_s, and can be defined as (Lee & Tien (1981); Mullins & Williams (1987))

$$C_1 = \frac{1}{c} \frac{36 \pi n \, p \, C_s}{(n^2 - p^2 + 2)^2 + 4 n^2 p^2} = 9.859475 \times 10^{-9} \, C_s \quad \text{with} \quad n = 2, \, p = 0.40 \,. \tag{2.8}$$

The mean absorption coefficients, derived in Ripoll *et al.* (2001), take this frequency dependence of the opacity of the medium into account. They represent the opacity at a macroscopic level and have a strong influence on radiative heat transfer (Siegel & Howell (2001)). The mean absorption coefficients are given by

$$\sigma_P = 360 \; C_1 \frac{k \zeta_5}{\pi^4 h} T = C_P \, T \quad \text{with} \quad C_P = 360 \frac{k \zeta_5}{\pi^4 h} C_1 \tag{2.9}$$

$$\sigma_E = \; 3 \sigma_P \frac{1 + \|A\|^2}{B (3 + \|A\|^2)(1 - \|A\|^2)} \quad \text{and} \quad \sigma_F = \frac{\sigma_P}{4} \frac{5 + \|A\|^2}{B (1 - \|A\|^2)}, \tag{2.10}$$

with $\zeta_5 = 1.03692$. $\vec{A}$ and B are defined as

$$\vec{A} = \frac{2 - \sqrt{4 - 3 \|f\|^2}}{\|f\|^2} \vec{f} \quad \text{and} \quad B = \frac{T}{T_R} \left[\frac{3 + \|A\|^2}{3(1 - \|A\|^2)^3} \right]^{\frac{1}{4}} . \tag{2.11}$$

3. Simplifications of the M_1-model with mean absorption coefficients

3.1. *Expansion of the absorption coefficients*

To simplify the effective mean coefficients σ_E and σ_F, first the expression for B, given in (2.11), is introduced into (2.10), such that σ_E and σ_F are functions of $\|f\|$ only through

A. Since A tends to zero for small $\|f\|$, with (2.11) we then write A as a second order Taylor series expansion for small $\|f\|$, which is given by

$$\|A\| = 3/4\|f\| + O(f^3)\,. \tag{3.1}$$

After developing σ_E and σ_F in a Taylor series expansion for small A and replacing A using (3.1), we obtain

$$\sigma_E = C_P\, G_E(f)\, T_R\,, \tag{3.2}$$

$$\sigma_F = C_P\, G_F(f)\, T_R\,, \tag{3.3}$$

with

$$G_E(f) = 1 + \frac{15}{32}\|f\|^2 + O(\|f\|^4) \tag{3.4}$$

and

$$G_F(f) = \frac{5}{4}\left(1 + \frac{33}{200}\|f\|^2 + O(\|f\|^4)\right)\,. \tag{3.5}$$

The isotropic limit for these coefficients can be obtained taking $\|f\| = 0$ in (3.4) and (3.5), which leads to $G_E \simeq 1$ and $G_F \simeq 5/4$. For the mean absorption coefficients in the isotropic limit follows

$$\sigma_E = C_P\, T_R \quad \text{and} \quad \sigma_{\mathrm{F}} = 5/4\, \mathrm{C_P\, T_R}\,. \tag{3.6}$$

3.2. *Expansion of the Eddington tensor*

The Eddington tensor D_R has a complex form, which leads to various problems. For instance, the Jacobian matrix and the eigenvalues cannot be expressed easily for multi-dimensional problems. Then, the development of numerical schemes, particularly of implicit methods, is not straight forward. Even in one dimension, the Eddington tensor has to be treated in a special way, as, for instance, in the numerical scheme proposed by Brunner & Holloway (2001). Moreover, if an averaged form of the M_1-model is being developed, this tensor must be simplified without modifying its main properties. Here, the Eddington tensor is expanded in a Taylor series around the directional equilibrium $f = 0$ and around the anisotropic limit $f = 1$. The two limits are then connected.

Combining (2.4) and (2.11) leads to $\chi(A) = (1 + 3\|A\|^2)/(3 + \|A\|^2)$. With this expression, the Eddington tensor (2.3) can be rewritten as

$$\vec{\vec{D}}_R \;=\; \frac{1 - \|A\|^2}{3 + \|A\|^2}\vec{\vec{\mathrm{Id}}} + \frac{4\|A\|^2}{3 + \|A\|^2}\vec{n} \otimes \vec{n}\,. \tag{3.7}$$

Expanding the Eddington tensor of the M_1-model as given by (3.7) for small $\|A\|$ and then replacing $\|A\|$ by Eq. (3.1) leads to

$$\vec{\vec{D}}_R \simeq \frac{1}{3}\left[(1 - \frac{3}{4}\|f\|^2)\vec{\vec{\mathrm{Id}}} + \frac{9}{4}\|f\|^2\vec{n} \otimes \vec{n} + O(\|f\|^4)\right]\,. \tag{3.8}$$

An even more simplified form of the Eddington tensor can be achieved by considering only the diagonal contributions of both terms in (3.8), i.e. $(D_R^{a,b})_{a,b=x,y} \simeq (D_R^{a,a})_{a=x,y}$. This leads to the following approximation

$$\vec{\vec{D}}_R \simeq \frac{1}{3}\left[1 + \frac{3}{2}\|f\|^2 + O(\|f\|^4)\right]\vec{\vec{\mathrm{Id}}}\,. \tag{3.9}$$

Similar to the expansions for the mean absorption coefficients, also here it is obvious that these expansions for small $\|f\|$ cannot describe the anisotropic limit. It can easily

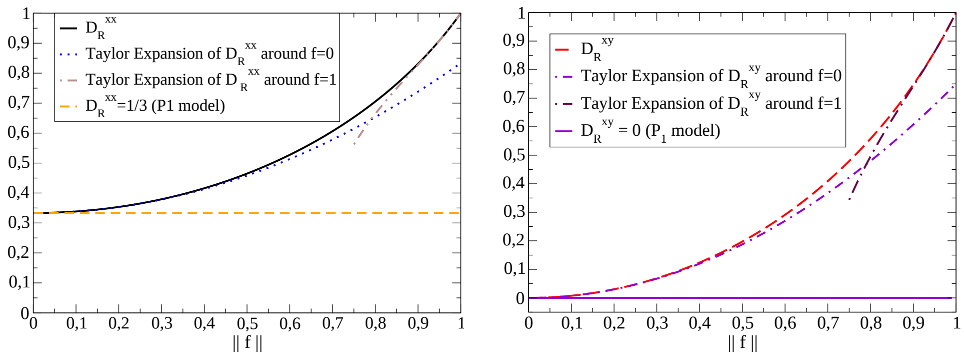

FIGURE 1. Left: Diagonal component D_R^{xx} of the Eddington tensor D_R and its Taylor series expansions. Right: Deviatoric component D_R^{xy} of the Eddington tensor D_R and its Taylor series expansions

be seen in (2.3) that, in the anisotropic limit, when f goes to 1, the first part of this tensor is zero, and that the second part tends to $f \otimes f$. Here, this property is lost and the diagonal part does not become zero in this limit. Hence, this model is not able to describe strong disequilibrium effects. This can be seen in Fig. 1, where the components of the Eddington tensor and their Taylor expansions are plotted.

However, this limit can be described by an expansion of the Eddington tensor for $\|f\| \to 1$. Again, since $\|A\| = 1$ for $\|f\| = 1$, we first expand (3.7) for $\|A\| \to 1$, and then replace $\|A\|$ by the expansion of $\|A\|$ for $\|f\| \to 1$, given by

$$\|A\| = 1 + 2\left(\|f\| - 1\right) + 4\left(\|f\| - 1\right)^2 + O\left(\left(\|f\| - 1\right)^3\right) . \tag{3.10}$$

The resulting expression for the Eddinton tensor in the limit $\|f\| \to 1$ is

$$\vec{\vec{D}}_R \simeq \vec{n} \otimes \vec{n} + (\vec{\vec{\mathrm{Id}}} - 3\vec{n} \otimes \vec{n})(-6\|f\|^3 + 16\|f\|^2 - 15\|f\| + 5) + O\left((\|f\| - 1)^4\right) . \tag{3.11}$$

It is shown in Fig. 1 that the Eddington tensor can be approximated by the two Taylor series expansions obtained for small $\|f\|$ and for $\|f\| \to 1$. To achieve good accuracy, the third order of (3.11) has to be retained.

4. Averaged M_1-model with mean absorption coefficients

The main purpose here is to develop an ensemble-averaged formulation of the radiation model, which accounts for turbulence-radiation interactions, but is still not too complex or numerically costly, so that it can be used in fire simulations. An averaged form of the M_1-model with mean absorption coefficients has already been derived by Ripoll (2002). However, because of the complexity of the averaged quantities, this model cannot be applied directly in numerical simulations. Here, a simplified form of this model will be derived.

The following mean quantities are introduced:

$$\overline{T} = \int_{\mathcal{D}_T} T\,\mathcal{P}_T(T)\,dT\,, \qquad \overline{T}_R = \int_{\mathcal{D}_{T_R}} T_R \mathcal{P}_{T_R}(T_R) dT_R\,, \tag{4.1}$$

$$\overline{f_i} = \int_{\mathcal{D}_{f_i}} f_i \, \mathcal{P}_{f_i}(f_i)\, df_i, \quad \forall i = x, y, z\,, \quad \text{and} \quad \overline{C}_s = \int_{\mathcal{D}_{C_s}} C_s \mathcal{P}_{C_s}(C_s) dC_s\,, \tag{4.2}$$

where the integration domains are given as $\mathcal{D}_T = \mathcal{D}_{T_R} =]-\infty, +\infty[$, $\mathcal{D}_f =]-1, 1[$, and $\mathcal{D}_{C_s} =]0, 1[$. The probability density functions $\mathcal{P}_T(T)$, $\mathcal{P}_{T_R}(T_R)$, $\mathcal{P}_{C_s}(C_s)$, and $\mathcal{P}_{f_i}(f_i)$, $\forall i = x, y, z$ are assumed to be given by the following Gaussian and β functions:

$$\mathcal{P}_T(T) = \frac{1}{\sqrt{2\pi \overline{T'T'}}} e^{-\frac{(T-\overline{T})^2}{2\overline{T'T'}}}\,, \qquad \mathcal{P}_{T_R}(T_R) = \frac{1}{\sqrt{2\pi \overline{T_R' T_R'}}} e^{-\frac{(T_R-\overline{T}_R)^2}{2\overline{T_R' T_R'}}}\,, \tag{4.3}$$

$$\mathcal{P}_{f_i}(f_i) = \frac{(f_i+1)^{\alpha_{f_i}-1}(1-f_i)^{\beta_{f_i}-1}}{2^{\alpha_{f_i}+\beta_{f_i}-1}} \frac{\Gamma(\alpha_{f_i}+\beta_{f_i})}{\Gamma(\alpha_{f_i})\Gamma(\beta_{f_i})}, \quad \forall i = x, y, z\,, \tag{4.4}$$

$$\mathcal{P}_{C_s}(C_s) = (C_s)^{\alpha_s - 1}(1-C_s)^{\beta_s - 1} \frac{\Gamma(\alpha_s+\beta_s)}{\Gamma(\alpha_s)\Gamma(\beta_s)} \tag{4.5}$$

$$\text{with} \qquad \alpha_{f_i} = \overline{f_i}\gamma_{f_i}\,, \quad \beta_{f_i} = (1-\overline{f_i})\gamma_{f_i}\,, \quad \gamma_{f_i} = \frac{\overline{f_i}(1-\overline{f_i})}{\overline{f_i' f_i'}} - 1, \;\; \forall i = x, y, z\,, \tag{4.6}$$

$$\alpha_s = \overline{C}_s\gamma_s\,, \quad \beta_s = (1-\overline{C}_s)\gamma_s\,, \quad \gamma_s = \frac{\overline{C}_s(1-\overline{C}_s)}{\overline{C_s' C_s'}} - 1\,, \quad \Gamma(x) = \int_0^\infty e^{-t} t^{(x-1)} dt\,. \tag{4.7}$$

The direct integration of the Gaussian functions leads to the moments of T_R and T in the following form

$$\begin{aligned}
\overline{X^9} &= 945\, \overline{X'X'}^4\, \overline{X} + 1260\, \overline{X'X'}^3\, \overline{X}^3 + 378\, \overline{X'X'}^2\, \overline{X}^5 + 36\, \overline{X'X'}\, \overline{X}^7 + \overline{X}^9, \\
\overline{X^8} &= 105\, \overline{X'X'}^4 + 420\, \overline{X'X'}^3\, \overline{X}^2 + 210\, \overline{X'X'}^2\, \overline{X}^4 + 28\, \overline{X'X'}\, \overline{X}^6 + \overline{X}^8, \\
\overline{X^5} &= 15\, \overline{X'X'}^2\, \overline{X} + 10\, \overline{X'X'}\, \overline{X}^3 + \overline{X}^5, \\
\overline{X^4} &= 3\, \overline{X'X'}^2 + 6\, \overline{X'X'}\, \overline{X}^2 + \overline{X}^4\,,
\end{aligned} \tag{4.8}$$

where X stands for T_R or T, and $\overline{X'X'}$ for $\overline{T_R' T_R'}$ or $\overline{T'T'}$.

To obtain a closed form of the averaged equations, two assumptions have to be made in the following. First, we assume that the soot volume fraction is uncorrelated from the radiative energy and flux and from the matter temperature. This assumption can be justified for fires, considering the experimental results given by Coppalle & Joyeux (1994). Note however, that correlations of the radiative properties of soot and other quantities are retained.

Secondly, it is assumed that the anisotropic factor and the radiative temperature are uncorrelated. This assumption is difficult to justify, although in the limit, where radiation is isotropic and the anisotropic factor tends to zero, also the correlation becomes small. Note however, that the assumption of uncorrelated anisotropic factor and radiative temperature does not imply that radiative flux and radiative energy are uncorrelated, since $\overline{E_R F_R} = c\overline{f}\, \overline{E_R^2} \neq \overline{E}_R\, \overline{F}_R$.

According to the definition of the ensemble averages and the above assumptions, the mean radiative energy and flux can be determined as

$$\overline{E}_R = \overline{aT_R^4} = \int_{\mathcal{D}_{T_R}} aT_R^4 \mathcal{P}_{T_R}(T_R) dT_R \quad \text{and} \quad \overline{F}_R = c\overline{f}\; \overline{E}_R\,. \tag{4.9}$$

It is convenient to introduce turbulent effective mean absorption coefficients defined as

$$\sigma_P^t = \frac{\overline{\sigma_P T^4}}{\overline{T}^4} = \overline{C}_P \, \frac{\overline{T^5}}{\overline{T}^4} \,, \tag{4.10}$$

$$\sigma_E^t = \frac{\overline{\sigma_E E_R}}{\overline{E}_R} = \overline{C}_P \, \overline{G}_E \, \frac{\overline{T_R^5}}{\overline{T_R^4}} \,, \quad \text{and} \quad \sigma_F^t = \frac{\overline{\sigma_F F_R}}{\overline{F}_R} = \overline{C}_P \, \frac{\overline{G_F f}}{\overline{f}} \, \frac{\overline{T_R^5}}{\overline{T_R^4}} \,. \tag{4.11}$$

Then, the averaged M_1-model with mean absorption coefficients can be written as

$$\partial_t \overline{E}_R + \nabla \cdot \overline{F}_R = c\big[\sigma_P^t a \overline{T}^4 - \sigma_E^t \overline{E}_R\big] \,, \tag{4.12}$$

$$\frac{1}{c}\partial_t \overline{F}_R + c \, \nabla \cdot \, \big(\overline{D}_R(f) \, \overline{E}_R\big) = -\sigma_F^t \, \overline{F}_R \,, \tag{4.13}$$

where for $a, b = x, y, z$

$$\overline{D}_R^{ab}(f) = \int_{\mathcal{D}_f} D_R^{ab}(f_x, f_y, f_z)\mathcal{P}_f(f) df \,. \tag{4.14}$$

Here, $P_f(f)$ is the joint pdf of f_x, f_y, f_y, which can in principle be modeled as a multivariate β-function, depending on the mean components and the variances and co-variances of f_x, f_y, and f_y. These can be computed at shown below. However, since the evaluation of this pdf is very complex, the further assumption that the components of the anisotropy factor are uncorrelated leads to

$$\overline{D}_R^{ab}(f) = \int_{\mathcal{D}_{f_x}} \int_{\mathcal{D}_{f_y}} \int_{\mathcal{D}_{f_z}} D_R^{ab}(f_x, f_y, f_z)\mathcal{P}_{f_x}(f_x)\mathcal{P}_{f_y}(f_y)\mathcal{P}_{f_z}(f_z) \, df_x \, df_y \, df_z \,, \tag{4.15}$$

where the pdfs of the individual components can be modeled according to (4.4).

This system is closed, if the variances of the radiative energy and of the anisotropic factor are known. The variance of the anisotropic factor only appears in the expressions for $\overline{G}_E$, $\overline{G}_F$, and $\overline{D}_R$. If the variance of the anisotropic factor is assumed to be small, it follows that only the variances of the radiative energy is needed. Indeed, if $\overline{f^{a\prime} f^{a\prime}} \simeq 0$, $\forall a = x, y, z$, then $\overline{G}_E(f) \simeq G_E(\overline{f})$, $\overline{G}_F(f) \simeq G_F(\overline{f})$, and $\overline{D}_R(f) \simeq D_R(\overline{f})$. This assumption will be discussed in section 5.2. The model then becomes

$$\partial_t \overline{E}_R + \nabla \cdot \overline{F}_R = c\overline{C}_P \left(a\overline{T^5} - aG_E(\overline{f})\overline{T_R^5}\right) , \tag{4.16}$$

$$\frac{1}{c}\partial_t \overline{F}_R + c \, \nabla \cdot D_R(\overline{f})\overline{E}_R = -c\overline{C}_P \, G_F(\overline{f}) \, a\overline{T_R^5} \, \overline{f} \,. \tag{4.17}$$

Similarly to the derivation of the diffusion formulation of the M_1-model given by (2.6) and (2.7), an averaged diffusion formulation can be obtained from (4.12) and (4.13). The diffusion equation for the mean radiative flux then becomes

$$-\vec{\nabla} \cdot (\frac{\overline{D}_R(f)}{\sigma_E^t} \, \vec{\nabla} \cdot \overline{F}_R) + \sigma_F^t \overline{F}_R = -c\vec{\nabla} \cdot (\frac{\sigma_P^t}{\sigma_E^t} \overline{D}_R(f) a \overline{T}^4) \,. \tag{4.18}$$

5. Model for the variances of the radiative variables

In the averaged M_1-model, given by (4.12) and (4.13), the variance of both the radiative temperature and the anisotropy appear, and models for these quantities have to be provided. Expressions for the variances have been derived by Ripoll (2002). Here, simplified formulations for these quantities will be developed.

5.1. *General formulation*

Using the assumption made in the previous section that the radiative energy and the anisotropy factor are uncorrelated, the variances of the radiative variables can be written as

$$\overline{E'_R E'_R} = \overline{(E_R - \overline{E}_R)^2} = \overline{E^2_R} - \overline{E}^2_R\,, \tag{5.1}$$

$$\overline{F'_R F'_R} = \overline{(cfE_R - \overline{cfE_R})^2} = \overline{(cfE_R - c\overline{f}\ \overline{E_R})^2} = c^2\overline{f^2}\ \overline{E^2_R} - c^2\overline{f}^2\ \overline{E}^2_R\,. \tag{5.2}$$

Introducing $\overline{f'f'} = \overline{f^2} - \overline{f}^2$ into (5.2), leads to an expression relating the variances of the radiative flux, the anisotropy factor, and the radiative energy as

$$\overline{F'_R F'_R} = c^2\,\overline{f'f'}\,\overline{E^2_R} + c^2\,\overline{f}^2\,\overline{E'_R E'_R}\,. \tag{5.3}$$

Ripoll (2002) has derived transport equations for the variances of radiative energy and radiative flux. However, in their general form, mainly because of the different integral terms of the Eddington tensor, these equations are complex and not easily applicable. If in the variance equation of the radiative flux, the directional equilibrium assumption is applied for the Eddington tensor, and if, according to $\overline{\|f\|} \longrightarrow 0$ in (3.4) and (3.5), $\overline{G}_E \simeq 1$ and $\overline{G}_F \simeq 5/4$, the equations for $\overline{E'_R E'_R}$ and $\overline{F'_R F'_R}$ become

$$\frac{1}{2}\partial_t\overline{E'_R E'_R} + c\nabla\cdot(\overline{E'_R E'_R}\ \overline{f}) - \frac{c}{2}\overline{f}\cdot\nabla\overline{(E'_R E'_R)} =$$
$$c\overline{C}_P(a^2\overline{T^9} + \frac{15}{32}a^2\overline{T^9}\,\overline{\|f^2\|} - a\overline{T^5}\ \overline{E}_R) - c\overline{C}_P(\ a^2\overline{T^9_R} -\ a\overline{T^5_R}\ \overline{E}_R)\,, \tag{5.4}$$

$$\frac{1}{c}\partial_t\overline{F'_R F'_R} + \frac{c^2}{3}\overline{f}\,\nabla\overline{E'_R E'_R} = -c^2\frac{5}{2}\overline{C}_P(\ \overline{f^2}\ a^2\overline{T^9_R} - \overline{f}^2\ a\overline{T^5_R}\ \overline{E}_R)\,. \tag{5.5}$$

5.2. *Simplification around the equilibrium*

With (5.4) and (5.5), in three-dimensional simulations, four equations need to be solved to describe the spatial distribution of the variances of the radiative energy and the components of the radiative flux.

A major simplification can be achieved by assuming that the variance of the anisotropic factor is negligible. This implies that $\overline{f_a}^2 = \overline{f}^2_a, \forall\, a = x, y, z$, and hence the variance of the radiative flux can be expressed by the variance of the radiative temperature as $\overline{F^{a\prime}_R F^{a\prime}_R} = c\overline{f}^2_a\ \overline{E'_R E'_R},\ \forall\, a = x, y, z$. This assumption has already been used in section 4 to simplify the mean absorption coefficients and the Eddington tensor. It is noteworthy that neglect the variance of the anisotropy factor is not equivalent to neglect the variance of the radiative flux.

It can be shown that this assumption also implies that $\overline{\|f^2\|} = \|\overline{f}\|^2$, which also simplifies the second term on the right hand side in the equation for the radiative energy (5.4), leading to

$$\frac{1}{2}\partial_t\left(\overline{E'_R E'_R}(1 + 3\|\overline{f}\|^2)\right) + c\nabla\cdot(\overline{E'_R E'_R}\ \overline{f}) = c\overline{C}_P(a^2\overline{T^9} + \frac{15}{32}a^2\overline{T^9}\,\|\overline{f}\|^2 - a\overline{T^5}\ \overline{E}_R)$$
$$- c\overline{C}_P(1 + \frac{15}{4}\|\overline{f}\|^2)(a^2\overline{T^9_R} - a\overline{T^5_R}\ \overline{E}_R)\,. \tag{5.6}$$

This equation is now closed. The radiative energy is known from the solution of the equation for the mean radiative temperature, the matter temperature and the soot volume fraction are given by the flow solver, and averages of powers of the radiative temperature can be obtained from (5.1), (4.8), and definition of the radiative temperature (2.5).

5.3. *Algebraic model for the variance of the radiative energy*

Solving the transport equation for the variance of the radiative energy (5.6) can be avoided by introducing further simplifications. If the equation for the variance of the radiative energy is non-dimensionalized with the speed of light and a characteristic opacity σ, all terms are of the same order. This shows that the time needed to achieve a steady state scales with $(\sigma c)^{-1}$, which is typically much smaller than the flow time scales that perturb the steady state of (5.6). The unsteady term in the variance equations can therefore be neglected.

If it is assumed that production is equal to dissipation in the equation for the variance, an algebraic expression for the radiative temperature can be obtained as

$$\overline{T^9}(1+\frac{15}{32}\|\overline{f}\|^2)-(1+\frac{15}{4}\ \|\overline{f}\|^2)\overline{T_R^9}+(1+\frac{15}{4}\ \|\overline{f}\|^2)\,\overline{T_R^4}\,(\overline{T_R^5}-\overline{T^5})=0\,, \tag{5.7}$$

where the definition of the radiative temperature (2.5) has been used. This leads in the limit $\|f\|\longrightarrow 0$ to

$$\overline{T^9}-\overline{T_R^9}+(\overline{T_R^5}\ -\overline{T^5})\ \overline{T_R^4}=0\,. \tag{5.8}$$

Using (4.8), the algebraic model (5.7) can be written in a polynomial form as

$$A\ \overline{T_R'T_R'}^4+B\ \overline{T_R'T_R'}^3+C\ \overline{T_R'T_R'}^2+D\ \overline{T_R'T_R'}+E=0 \tag{5.9}$$

with

$$A=-900\,(1+\frac{15}{4}\|\overline{f}\|^2)\overline{T}_R\,,\qquad B=-1140\,(1+\frac{15}{4}\|\overline{f}\|^2)\overline{T}_R^3\,, \tag{5.10}$$

$$C=-300\,(1+\frac{15}{4}\|\overline{f}\|^2)\overline{T}_R^5-3\overline{T^5}\,,\quad E=\overline{T^9}(1+\frac{15}{32}\,\|\overline{f}\|^2)-\overline{T^5}\,\overline{T}_R^4\,, \tag{5.11}$$

$$D=-20\,(1+\frac{15}{4}\,\|\overline{f}\|^2)\,\overline{T}_R^7-6\,\overline{T^5}\,\overline{T}_R^2\,. \tag{5.12}$$

This algebraic model is easy to solve and can be pre-tabulated in terms of $\overline{T}$, $\overline{T}_R$, $\overline{T'T'}$, and $\|\overline{f}\|$. In the following we will demonstrate the consistency of this model in some relevant limits. To fully assess the validity of the algebraic model, which is based on equilibrium assumptions, it will have to be compared with solutions of the variance transport equation (5.6).

5.3.1. *Case* $\|\overline{f}\|=0$

Results from the solution of (5.9) for $\|\overline{f}\|=0$ and $\overline{T}=2000\,\mathrm{K}$ are shown in Fig. 2. It can be observed that for any combination of the parameters a positive solution for $\overline{T_R'T_R'}$ is obtained as long as $0\le\overline{T}_R\le\overline{T}$. Three comments can be made regarding Fig. 2. Firstly, when $\overline{T}\ne\overline{T}_R$, there exists a non-zero positive $\overline{T_R'T_R'}$, which is always larger than $\overline{T'T'}$, even if $\overline{T'T'}=0$. Secondly, both variances of radiative temperature and matter temperature are equal when $\overline{T}=\overline{T}_R$, which is shown by the solid line. This is consistent with the radiative equilibrium in the instantaneous M_1-model. Finally, when $\overline{T}\ne\overline{T}_R$ nonlinear solutions are obtained.

Even simpler models for the variance of the radiative temperature could be constructed from (4.8) by assuming that some higher moments of the radiative temperature and the matter temperature are equal. To assess this assumption, results from the algebraic model (5.8), denoted "$A1$" are shown for two values of the mean radiative temperature, $\overline{T}_R=1900\,\mathrm{K}$ and $1700\,\mathrm{K}$ in Fig. 2. Also shown are two simple approximations given by

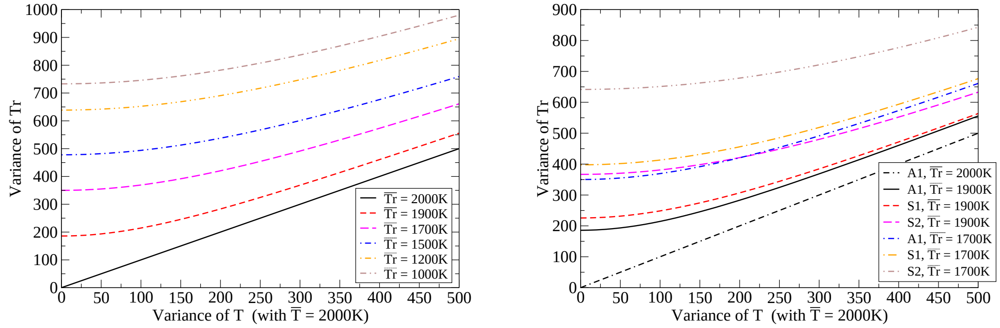

FIGURE 2. Left: solution of the algebraic model for $\|\overline{f}\| = 0$. Right: comparison of the algebraic model with other moment equations.

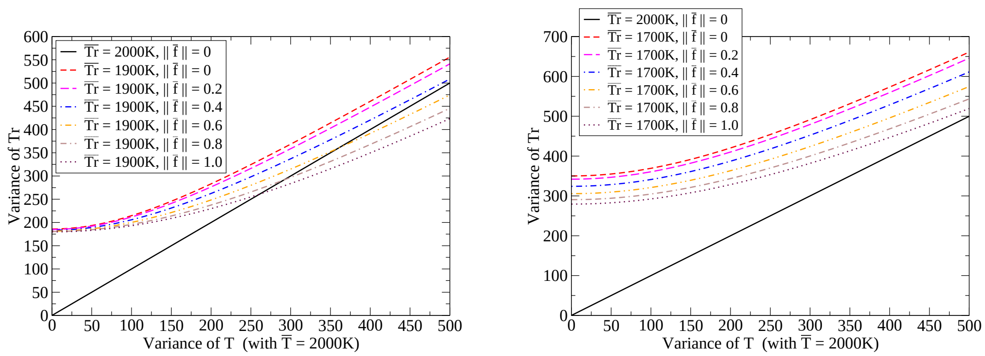

FIGURE 3. Solution of the algebraic model for different values of $\|\overline{f}\|$ with $\overline{T}_R = 1900\,\mathrm{K}$ (left) and $\overline{T}_R = 1700\,\mathrm{K}$ (right).

$\overline{T_R^9} = \overline{T^9}$ and $\overline{T_R^4} = \overline{T^4}$, which are denoted as "$S1$" and "$S2$", respectively. The solution of "$A1$" for $\overline{T} = \overline{T}_R = 2000\,\mathrm{K}$, implying $\overline{T'T'} = \overline{T'_RT'_R}$ is also shown, since it could also be used as a simple approximation for the variance of the radiative temperature.

It appears that model "$S2$" largely overpredicts the variance, while model "$S1$" yields a variance approximately 50 K too high, if compared to the algebraic model. It can hence be concluded that the algebraic equation should be used, since it is not more difficult to solve than the simple models.

5.3.2. *Case* $\|\overline{f}\| \neq 0$

Results from the solution of the algebraic model (5.7) with $\|\overline{f}\| \neq 0$ are given in Fig. 3 for two different values of the radiative temperature, $\overline{T}_R = 1700\,\mathrm{K}$ and $1900\,\mathrm{K}$, a variation of the anisotropic factor from $\|\overline{f}\| = 0$ to $\|\overline{f}\| = 1$, and a matter temperature of $T = 2000\,\mathrm{K}$. Again, it is obvious that positive solutions for the variance of the radiative temperature exist throughout the entire parameter range.

It is interesting to note that for stronger anisotropic disequilibrium ($\|f\| \neq 0$), the variance of the radiative temperature becomes smaller, while it becomes larger for stronger energetic disequilibrium ($T_R \neq T$).

6. Coupling with the Navier-Stokes equations

In the previous sections, a closed form of the averaged M_1-model with mean absorption coefficients has been presented, where closure has been introduced at various levels, such that models of different complexity and accuracy can be used. The only remaining unclosed terms are the mean matter temperature and its variance and the mean soot volume fraction. These quantities have to be provided from a combustion model, which is a part of the flow solver. Most combustion models, such as flamelet models (Peters (1984); Pitsch *et al.* (2000)), conditional moment closure models (Klimenko & Bilger (1999)), or pdf transport models (Pope (1985)) would allow to compute these quantities. However, most combustion models compute for Favre-averaged quantities, while the present formulation of the radiation model is based on Reynolds-averages. However, if the density is known, the appropriate pdfs can be converted to yield either Favre-averaged or Reynolds-averaged quantities. As an example, using a flamelet model and neglecting the variance of the scalar dissipation rate, the Favre-averaged temperature would be computed according to

$$\widetilde{T} = \int_0^1 T(Z)\widetilde{P}(\widetilde{Z}, \widetilde{Z''^2})dZ\,, \tag{6.1}$$

where Z is the mixture fraction, and the tilde denotes Favre-averages. Since the Favre pdf is defined as $\widetilde{P}(Z; \widetilde{Z}, \widetilde{Z''^2}) = \rho(Z)P(Z; \overline{Z}, \overline{Z''^2})/\overline{\rho}$ with ρ being the density, the Reynolds averaged temperature can be obtained as

$$\overline{T} = \int_0^1 T(Z)\frac{\overline{\rho}}{\rho(Z)}\widetilde{P}(\widetilde{Z}, \widetilde{Z''^2})dZ\,. \tag{6.2}$$

Using other combustion models, the appropriate quantities can be obtained accordingly.

7. Conclusions

In this paper, an ensemble-averaged version of the M_1 radiation model with mean absorption coefficients is proposed for describing radiation in large sooting flames. Closure is provided from transport equations for the variances of the radiative quantities, presumed pdf assumptions, and the assumption that the anisotropic factor and the radiative temperature are uncorrelated. This latter assumption is equivalent to the uncoupling the directional and energetic disequilibrium and seems to be a reasonable way to provide a closed and usable form of an averaged macroscopic radiative model.

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