Available online at www.sciencedirect.com
ScienceDirect
International Journal of Heat and Mass Transfer 51 (2008) 5008–5017
International Journal of HEAT and MASS TRANSFER
www.elsevier.com/locate/ijhmt

New aspects of the diffusion approximation for radiative transfer

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Received 9 January 2006; received in revised form 12 November 2007
Available online 21 April 2008

Abstract

The diffusion approximation is generalized to arbitrary locally isotropic participating media. It proves to be an approximate special solution of the full equation of radiative transfer accounting for absorption, scattering, and emission. This special solution must be completed with a solution of the radiative transfer equation without emission term in order to match the boundary conditions for the radiative field. Applied to combined heat and radiative transfer this scheme offers distinct computational advantages and broad applicability. Following these ideas a simple and robust method for one-dimensional radiation–conduction computations is constructed and verified.

Keywords: Radiative transport; Participating media; Diffusion approximation; Heat conduction

1. Introduction

Thermal radiative transport in gases, liquids and amorphous solids is well described by the equation of radiative transfer [1–3]. To find analytical or numerical solutions of the equation of radiative transfer is, in general, a task of considerable complexity even if additional simplifying assumptions as isotropic scattering, gray materials etc. are taken [1,4,5]. It is, therefore, gratifying that, with the Rosseland or diffusion approximation [6], a simplifying approach was found to calculate, if not the complete radiation field, but at least the flow of the radiant energy characterizing the net energy exchange with the medium in the limit of high optical density. In this approximation, the flow of the radiant energy is proportional to the temperature gradient in the medium. The diffusion approximation is usually derived for isotropic scattering [6,7,1] but, considered as a phenomenological law, works quite well also in more general situations [8] at least for regions far from boundaries.

Near boundaries, the diffusion approximation for the radiative flow may be rather poor. From a principal point of view, an even more important shortcoming is that it does not allow to properly formulate the boundary conditions for the radiative field since it yields only a partial information about this quantity. This shortcoming is evident for the problem of combined heat conduction and radiative energy transport. The heat flow and the radiative energy flow in the diffusion approximation are both proportional to the temperature gradient. They both vanish on thermally isolated boundaries. The diffusion approximation can, therefore, not be the only contribution to the radiative flow in this situation. The partial information on the radiative field may appear sufficient if attention is paid not primarily to the radiative field in the participating medium but rather to the question how the presence of a participating medium influences the radiative energy exchange between material bodies. The radiative flow through the medium seems then to be the important quantity for which the diffusion approximation provides a useful approximation. However, satisfactory results are obtained only under certain rather restricting conditions [1, 15.3] and if the diffusion approximation is completed with suitable, self consistent boundary conditions for the radiative flow leading to jump boundary conditions for the temperature [7] at the boundary between two bodies in thermal contact and to a value of the temperature gradient different from zero at the boundaries of a participating and thermally isolated medium.

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0017-9310/$ - see front matter
doi:10.1016/j.ijheatmasstransfer.2008.01.029

Nomenclature

a	absorption coefficient (m^{-1})
A	absorption coefficient for two-flux model (m^{-1})
c_p	specific heat per volume for constant pressure ($J\,m^{-3}\,K^{-1}$)
C_1	first radiation constant, $C_1 = 1.190044 \times 10^{20}\,W\,m^{-2}\,nm^4\,sr^{-1}$
C_2	second radiation constant, $C_2 = 1.438769 \times 10^7\,nm\,K$
$\vec{e}$, $\vec{e}'$	unit vectors in three dimensions indicating directions
D_+, D_-	coefficients in solution of homogeneous two-flux equations, Eqs. (41) and (42), ($W\,m^{-2}$)
E_+, E_-	spectral radiance in positive/negative x-direction ($W\,m^{-2}\,nm^{-1}$)
F	spectral radiance integrated over 4π solid angle ($W\,m^{-2}\,nm^{-1}$)
h	enthalpy per volume ($J\,m^{-3}$)
$\vec{J}$	spectral radiative power flow ($W\,m^{-2}\,nm^{-1}$)
$\vec{J}_Q$	heat flow ($W\,m^{-2}$)
L	spectral radiance ($W\,m^{-2}\,nm^{-1}\,sr^{-1}$)
L_n	expansion functions of the special solution of the equation of radiative transfer, Eq. (15), ($W\,m^{-2}\,nm^{-1}\,sr^{-1}$)
N	incident radiative flux ($W\,m^{-2}$)
P_l	Legendre polynomial of degree l
q	emission term in two-flux equations, Eq. (40), ($W\,m^{-2}$)
R_N	residuum of the Nth approximation to a solution of the equation of radiative transfer, Eqs. (15) and (18), ($W\,m^{-2}\,nm^{-1}\,sr^{-1}$)
s	scattering coefficient (m^{-1})
S	scattering coefficient for two-flux model (m^{-1})
W	Eq. (43) (m^{-1})
$Y_{l,m}$	spherical harmonic of order l
$\vec{x}$, $\vec{y}$	position vectors (m)

Greek symbols

$\delta_{m',m}$	Kronecker symbol: $\delta_{m',m} = 1$ if $m' = m$, $\delta_{m',m} = 0$ if $m' \neq m$
∇	gradient operator
η	auxiliary quantity, Eq. (78)
θ	auxiliary quantity, Eq. (59)
κ_{hrt}	coefficient of heat and radiative transport, Eq. (35), ($J\,m^{-1}\,K^{-1}$)
κ_Q	coefficient of heat conduction ($J\,m^{-1}\,K^{-1}$)
λ	wavelength (nm)
ρ_1	reflectivity of thermostat, Eq. (49)
Φ	phase function (sr^{-1})
$\mathbf{\Phi}$	integral operator with kernel Φ
ϕ_l	eigenvalue of $\mathbf{\Phi}$, Eq. (4)
$\mathbf{\Psi}$	integral operator, Eq. (12), (m)
Ψ	kernel of the operator $\mathbf{\Psi}$, Eq. (11), ($m\,sr^{-1}$)
ψ_l	eigenvalue of $\mathbf{\Psi}$, Eq. (13), (m)
ψ_1^{eff}	inverse of Rosseland mean attenuation coefficient, Eq. (31), (m)
σ_B	Stefan–Boltzmann constant, $\sigma_B = 5.6605 \times 10^{-8}$ ($W\,m^{-2}\,K^{-4}$)
τ	difference to surface temperature (K)
$d\Omega(\vec{e})$	element of solid angle in direction $\vec{e}$ (sr)

Subscripts

bb	blackbody
rad	radiative
inc	incident

Superscripts

h	refers to the homogeneous equation of radiative transfer
i	refers to the inhomogeneous equation of radiative transfer
*	complex conjugate

A different view is taken in the present work. Here, the radiative field in the medium is considered as a distinct physical system that exchanges energy with the medium by absorption and emission of radiation and causes an energy flow different from a heat flow. The radiative field is determined by the equation of radiative transfer together with the boundary conditions for the field at the border of the participating medium, i.e. the value of the incident (spectral) irradiance. Additional boundary conditions for the temperature field are needed if heat conduction occurs in the medium. The focus here is not on the bodies confining the medium, and the sources of radiation outside the medium just yield a given incident light flux.

In this view, the solution of radiative heat transfer problems combined with heat conduction in the medium requires to discuss the solution theory of the equation of radiative transfer. An approximate special solution of the equation of radiative transfer for a given temperature distribution in the medium is sought by solving this equation iteratively (Section 2). The contribution of this special solution to the radiative flow is, to the lowest order, given by the diffusion approximation. With this derivation, it is shown that the validity of the diffusion approximation does not rest on the isotropy of scattering or on the isotropy of the radiation field as it is assumed in Refs. [7,1] but uniquely on the condition that the temperature gradient and its spatial variations do not significantly change within an absorption length for radiation. Near boundaries, however, the diffusion approximation usually not represents the total radiative flow but must be completed with the flow contribution originating from a solution of the homogeneous equation, the equation without emission term, which is needed to match the boundary conditions for the radiation field.

In Section 3, these ideas are used to formulate a consistent solution of the problem of combined heat conduction and radiative transport. The resulting computational scheme conserves the significant conceptual simplifications and computational advantages of the original diffusion approximation but avoids its internal inconsistencies.

For a numerical test of the diffusion approximation, understood in the above sense, stationary heat conduction and radiative transport in a gray slab with constant material properties are considered within the two-flux approximation of the radiative field [9,1,2] (Section 4). The slab is irradiated on one side and held at a constant temperature on the other side. The exact solution amounts to the integration of a system of two ordinary differential equations containing two free parameters (Section 5). These parameters are determined by matching two boundary conditions, one on every side of the slab. The numerical integration demands a generalized 'shooting' algorithm [10, chapter 17] which fails for optically thick layers. In contrast, the algorithm resulting from the diffusion approximation is numerically robust and much faster for any physically reasonable set of material parameters. Its results coincide with the exact solution within a few percents for low values of the absorption coefficient and within less than one percent for higher values.

2. An approximate special solution of the equation of radiative transfer

The stationary equation of radiative transfer [1,2] expresses energy conservation for the radiant energy flow and reads in an operator notation as follows:

$$\vec{e}\cdot\nabla L = -(a+s)L + s\mathbf{\Phi}L + aL_{\mathrm{bb}}, \tag{1}$$

where $L(\vec{x},\vec{e},\lambda)$ is the spectral radiance which depends on the position $\vec{x}$, the direction of light propagation $\vec{e}$, $||\vec{e}|| = 1$, and the wavelength λ. The quantity $a(\vec{x},\lambda)$ denotes the absorption coefficient, $s(\vec{x},\lambda)$ the scattering coefficient. $\mathbf{\Phi}$ is an integral operator

$$\mathbf{\Phi} : f(\vec{e}) \rightarrow \oint \mathrm{d}\Omega(\vec{e}\,')\Phi(\vec{e},\vec{e}\,')f(\vec{e}\,'), \tag{2}$$

whose kernel $\Phi(\vec{x},\vec{e},\vec{e}\,',\lambda)$ is the phase function characterizing the scattering properties of the system. All material properties may depend explicitly on the local temperature $T(\vec{x})$. $L_{\mathrm{bb}}(T,\lambda)$ denotes the blackbody radiance given by

$$L_{\mathrm{bb}}(T,\lambda) = \frac{C_1}{\lambda^5}\frac{1}{\mathrm{e}^{C_2/(\lambda T)}-1}, \tag{3}$$

where C_1 and C_2 are the first and the second radiation constant. In the following, the dependence on the wavelength λ is no longer explicitly indicated.

The phase function of an isotropic material is rotation invariant implying that it is a function of the scalar product $\vec{e}\cdot\vec{e}\,'$ only [2, 13.2]. This function may be expanded into Legendre polynomials P_l

$$\Phi(\vec{x},\vec{e},\vec{e}\,') = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\phi_l(\vec{x})P_l(\vec{e}\cdot\vec{e}\,') = \sum_{l=0}^{\infty}\phi_l(\vec{x})\sum_{m=-l}^{l}Y_{l,m}(\vec{e})Y^{*}_{l,m}(\vec{e}\,'), \tag{4}$$

where the addition theorem for the spherical harmonics $Y_{l,m}$ [11, p. 28]

$$P_l(\vec{e}\cdot\vec{e}\,') = \frac{4\pi}{2l+1}\sum_{m=-l}^{l}Y_{l,m}(\vec{e})Y^{*}_{l,m}(\vec{e}\,') \tag{5}$$

has been used for the last step, Y^* denoting the complex conjugate of Y. With this last step, the representation of the kernel Φ in terms of a complete system of eigenfunctions has been achieved.

The phase function is normalized to

$$\oint \mathrm{d}\Omega(\vec{e}\,')\Phi(\vec{x},\vec{e},\vec{e}\,',\lambda) = 1 \tag{6}$$

implying

$$\phi_0(\vec{x}) = 1. \tag{7}$$

As a consequence, a symmetric radiation field, as e.g. $L_{\mathrm{bb}}(T(\vec{x}))$, produces no scattering effects. Integration of Eq. (1) over all directions $\vec{e}$ yields, therefore

$$\nabla\cdot\vec{J}(\vec{x}) = a(\vec{x})[4\pi L_{\mathrm{bb}}(T(\vec{x})) - F(\vec{x})], \tag{8}$$

where

$$\vec{J}(\vec{x}) = \oint \mathrm{d}\Omega(\vec{e})\vec{e}L(\vec{x},\vec{e}) \tag{9}$$

is the spectral radiative flux of the radiation field and

$$F(\vec{x}) = \oint \mathrm{d}\Omega(\vec{e})L(\vec{x},\vec{e}) \tag{10}$$

is the product of the local light velocity in the medium with the total spectral energy density of the radiation field [1, 13-4] and [2, 9.9–9.10].

The equation of radiative transfer (1) is, in mathematical terms, a linear integral–differential equation for the spectral radiance L with a source term aL_{bb}. The difference of two solutions of this equation is a solution of Eq. (1) without the source term, the homogeneous equation. Therefore, the solution of Eq. (1) for given boundary conditions can be written as the superposition of a special solution of the full, inhomogeneous equation not necessarily fulfilling the boundary conditions and of a solution of the homogeneous equation. The first part accounts for the source while, with the second part, the actual boundary conditions for the radiation field are matched. The solution theory for the homogeneous equation is treated elsewhere in detail (see e.g. [3] and [4]) and will not be discussed here. We retain that such a solution is important only in a surface region within a few absorption lengths from the boundaries.

In order to find an approximation to a special solution in a systematic way we use $L_{bb} = \mathbf{\Phi} L_{bb}$ to get

$$L = L_{bb} - \mathbf{\Psi}\vec{e}\cdot\nabla L, \tag{11}$$

where $\mathbf{\Psi}$ is the operator

$$\mathbf{\Psi} = [a\mathbf{I} + s(\mathbf{I} - \mathbf{\Phi})]^{-1}. \tag{12}$$

The kernel Ψ of the operator $\mathbf{\Psi}$ has an expansion similar to the expansion of the kernel Φ

$$\Psi(\vec{x},\vec{e},\vec{e}') = \sum_{l=0}^{\infty}\psi_l(\vec{x})\sum_{m=-l}^{l}Y_{l,m}(\vec{e})Y^*_{l,m}(\vec{e}'), \tag{13}$$

with

$$\psi_l(\vec{x}) = \frac{1}{a(\vec{x}) + s(\vec{x})[1-\phi_l(\vec{x})]}. \tag{14}$$

Eq. (11) is equivalent to Eq. (1), i.e. a solution of Eq. (1) is a solution of Eq. (11) and vive versa, only if the operators $\mathbf{\Psi}$ and $\mathbf{\Psi}^{-1}$ exist. This is true if all expressions $a(\vec{x}) + s(\vec{x})[1-\phi_l(\vec{x})]$ are different from zero. Since always $\phi_0 = 1$, the following considerations do not apply if the absorption coefficient $a(\vec{x})$ goes to zero, i.e. when the medium does not significantly absorb but mainly scatters.

Eq. (11) implies that the radiation field $L^{\mathrm{i}} = L_{bb}(T_0)$ is a special solution of the inhomogeneous equation in a region where $T(\vec{x}) = T_0 = \text{const}$. If $T(\vec{x})$ is not constant but slowly varying with $\vec{x}$ iteratively solving Eq. (11) may provide an approximate solution of the inhomogeneous equation: inserting a Nth approximation $L^{(N)}$ into the right hand side of Eq. (11) gives the next approximation $L^{(N+1)}$. One starts with $L^{(0)} = L_{bb}$. This procedure is equivalent to write L^{i} as

$$L^{\mathrm{i}}(\vec{x},\vec{e}) = \sum_{n=0}^{N}L_n(\vec{x},\vec{e}) + R_N(\vec{x},\vec{e}), \tag{15}$$

with

$$L_0 = L_{bb}, \tag{16}$$

$$L_{n+1} = -\mathbf{\Psi}\vec{e}\cdot\nabla L_n \quad \text{for } n = 0,1,\ldots,N, \tag{17}$$

$$R_N = L_{N+1}(\vec{x},\vec{e}) - \mathbf{\Psi}\vec{e}\cdot\nabla R_N. \tag{18}$$

The first terms of the expansion Eq. (15) of the special solution L^{i} are easily calculated if we take into account that

$$\oint d\Omega(\vec{e}')\Psi(\vec{x},\vec{e},\vec{e}')f_l(\vec{e}') = \psi_l(\vec{x})f_l(\vec{e}) \tag{19}$$

for every function $f_l(\vec{e})$ which is a linear combination of spherical harmonics $Y_{l,m}(\vec{e})$ of a fixed degree l. This is a direct consequence of the expansion (13) of the kernel Ψ. Since $Y_{0,0}$ is the constant $\sqrt{\frac{1}{4\pi}}$, the components e_j of $\vec{e}$ are linear combinations of $Y_{1,m}$, and the components $e_je_k - \frac{1}{3}\delta_{j,k}$, $j,k = 1,2,3$ of the symmetric tensor with zero trace are linear combinations of the $Y_{2,m}$ one readily obtains

$$L_1(\vec{x},\vec{e}) = -\psi_1(\vec{x})\vec{e}\cdot\nabla L_{bb}(T(\vec{x})) \tag{20}$$

and

$$L_2(\vec{x},\vec{e}) = \sum_{j,k=1}^{3}\left[\psi_2(\vec{x})\left(e_je_k - \frac{1}{3}\delta_{j,k}\right) + \frac{1}{3}\psi_0(\vec{x})\delta_{jk}\right] \times\frac{\partial}{\partial_{x_j}}\left[\psi_1(\vec{x})\frac{\partial}{\partial_{x_k}}L_{bb}(T(\vec{x}))\right]. \tag{21}$$

Eq. (15) with the recursion (16) and (17) is an expansion of a special solution of the equation of radiative transfer in terms of inverse powers of the coupling parameters a, s, and Φ between radiation and matter. Higher order terms of this expansion can also be systematically calculated but involve always higher partial derivatives of $L_{bb}(T(\vec{x}))$ with respect to the space coordinates x_j and the decomposition into irreducible parts of always higher tensor products $e_{i_1}, e_{i_2}, \ldots, e_{i_n}$. The corresponding expressions soon become unduly complicated and one has to specify an ever increasing number of functions ψ_n restricting the practical usefulness of this expansion to the lowest orders.

The above considerations are applied to the problem of combined heat conduction and radiative energy transport in Section 3. There, the temperature field $T(\vec{x})$ is no longer a function given from outside but is determined by the differential equation for heat conduction including an interaction term with the radiation field and the boundary conditions for the temperature or the heat flow. Under these circumstances, it is natural to consider the series cut after the second term taking into account only L_0 and L_1. The error R_N committed by cutting a recursive series after N terms is of the order of the first neglected term L_{N+1}. Cutting the series after L_1 is, therefore, a valuable approximation if $|L_2| \ll |L_0 + L_1|$ which amounts to the condition

$$|\psi_1\psi_2|\left|\left(\vec{e}\cdot\nabla(\vec{e}\cdot\nabla L_{bb}) + \frac{s(1-\phi_2)}{3a}\Delta L_{bb}\right)\right| \ll |L_{bb} - \psi_1\vec{e}\cdot\nabla L_{bb}| \tag{22}$$

for constant material properties which is the generic case. It follows from the facts that the phase function is non-negative and the inequality $|P_l(\xi)| \leqslant 1$ for $|\xi| \leqslant 1$ [12, 5.4.4] that $1 - \Phi_l \geqslant 0$ and, therefore, that $\psi_l \geqslant 1/a$. As a consequence, condition (22) is fulfilled if the inequalities

$$\frac{1}{a}\left|\frac{\partial L_{bb}}{\partial x_i}\right| \ll L_{bb} \quad \text{and} \quad \frac{1}{a^2}\left|\frac{\partial^2 L_{bb}}{\partial x_i \partial x_j}\right| \ll L_{bb} \tag{23}$$

for $i,j = 1,2,3$ are valid, i.e. if the temperature field $T(\vec{x})$ and the components of ∇T do not appreciably change within a distance a^{-1}. This condition may be fulfilled even for small values of the absorption coefficient.

Calculating the quantities $\vec{J}$ and F from expansion (15) up to $N = 2$ yields

$$\vec{J}^{\mathrm{i}}(\vec{x}) = -\frac{4\pi}{3}\psi_1(\vec{x})\nabla L_{bb}(T(\vec{x})) \tag{24}$$

and

$$F^{\mathrm{i}}(\vec{x}) = 4\pi L_{bb}(T(\vec{x})) - \psi_0(\vec{x})\nabla\cdot\vec{J}^{\mathrm{i}}(\vec{x}). \tag{25}$$

Eq. (25) reproduces Eq. (8).

Eq. (24) is the diffusion approximation for the radiative flux. Its validity is bound to the conditions (23) and it is established here for arbitrary locally isotropic but not necessarily isotropically scattering media. It is argued (see e.g. [1]) that the diffusion approximation may fail near boundaries because the radiation field may be there far from symmetric. In fact, the field L^{i} is not far from symmetric if the diffusion approximation applies as a consequence of Eq. (23). However, the special solution L^{i} must be completed with the solution of the homogeneous equation, the equation without emission term, in order to match the boundary conditions for the total radiation field yielding an additional term to the radiative energy flow important only in the boundary region. The latter contribution and, hence, the total field may be far from symmetric depending on the reflectance of the sample and on the boundary conditions for the radiation field. But this asymmetry does not necessarily impair the validity of the diffusion approximation near boundaries, its validity being bound rather to the requirement that the inequalities (23) are fulfilled.

3. Combined heat conduction and radiative transport

Heat conduction and radiative transport are considered for a solid at rest. For an isobaric process, energy conservation is most easily expressed in terms of the enthalpy per volume h

$$\frac{\partial h}{\partial t} = c_p \frac{\partial T}{\partial t} = -\nabla \cdot \vec{J}_Q - \int_0^\infty \mathrm{d}\lambda \nabla \cdot \vec{J}, \tag{26}$$

where c_p denotes the specific heat per volume for constant pressure. The terms on the right hand side account for the change of the heat content of the volume element due to the heat flow $\vec{J}_Q$ and due to energy exchange with the radiative field.

For the heat flow, Fourier's law is assumed

$$\vec{J}_Q = -\kappa_Q \nabla T \tag{27}$$

κ_Q being the coefficient of heat conduction. The radiative energy flow

$$\vec{J}_{\mathrm{rad}}(\vec{x}) = \int_0^\infty \mathrm{d}\lambda \vec{J}(\vec{x}, \lambda) \tag{28}$$

is the sum of a flow due to the special solution of the inhomogeneous equation and of the flow due to the solution of the homogeneous equation

$$\vec{J}_{\mathrm{rad}} = \vec{J}^{\mathrm{i}}_{\mathrm{rad}} + \vec{J}^{\mathrm{h}}_{\mathrm{rad}}. \tag{29}$$

If the approximation Eq. (24) is inserted into Eq. (28) the radiative flow $\vec{J}^{\mathrm{i}}_{\mathrm{rad}}$ can be written as

$$\vec{J}^{\mathrm{i}}_{\mathrm{rad}}(\vec{x}) = -\frac{16}{3}\sigma_{\mathrm{B}} T^3(\vec{x}) \psi_1^{\mathrm{eff}}(\vec{x}, T(\vec{x})) \nabla T(\vec{x}). \tag{30}$$

Here σ_{B} denotes the Stefan–Boltzmann constant and ψ_1^{eff} is defined by

$$\psi_1^{\mathrm{eff}}(\vec{x}, T) = \frac{\int_0^\infty \mathrm{d}\lambda \psi_1(\vec{x}, \lambda, T) \frac{\partial}{\partial T} L_{\mathrm{bb}}(T, \lambda)}{\int_0^\infty \mathrm{d}\lambda \frac{\partial}{\partial T} L_{\mathrm{bb}}(T, \lambda)}, \tag{31}$$

with L_{bb} given by Eq. (3). The identity

$$\int_0^\infty \mathrm{d}\lambda L_{\mathrm{bb}} = \frac{1}{4\pi}\sigma_{\mathrm{B}} T^4 \tag{32}$$

has been used.

The result (30) corresponds to the one derived from the diffusion approximation the quantity $1/\psi_1^{\mathrm{eff}}$ being the local Rosseland mean attenuation coefficient [1, 15-3.2] now generalized to non-isotropically scattering media. But in contrast to previous treatments ([1, 15-4.2] and references therein), conservation of heat is now expressed by a completed equation

$$c_p \frac{\partial T}{\partial t}(\vec{x}, t) = \nabla \cdot [\kappa_{\mathrm{hrt}}(\vec{x}, T(\vec{x}, t)) \nabla T(\vec{x}, t)] + \int_0^\infty \mathrm{d}\lambda a(\vec{x}, T(\vec{x}, t), \lambda) \oint \mathrm{d}\Omega(\vec{e}) L^{\mathrm{h}}(\vec{x}, t, \vec{e}, \lambda), \tag{33}$$

where L^{h} is the solution of the homogeneous equation of radiative transfer with values

$$L^{\mathrm{h}}(\vec{x}, t, \vec{e}, \lambda) = L_{\mathrm{inc}}(\vec{x}, t, \vec{e}, \lambda) - L_{\mathrm{bb}}(T(\vec{x}, t), \lambda) - L_1(\vec{x}, t, \vec{e}, \lambda), \tag{34}$$

on boundary points $\vec{x}$ for all directions $\vec{e}$ of the incident radiation L_{inc}. The radiation field L_1 is given by Eq. (20); the contributions of L_2 and of higher order terms to the boundary conditions of L^{h} are neglected.

The coefficient

$$\kappa_{\mathrm{hrt}}(\vec{x}, T) = \kappa_Q(\vec{x}, T) + \frac{16}{3}\sigma_{\mathrm{B}} T^3 \psi_1^{\mathrm{eff}}(\vec{x}, T) \tag{35}$$

describes a combined effect of heat conduction and radiative transport. The function $\kappa_{\mathrm{hrt}}(\vec{x}, T)$ should, like the coefficient of heat conductivity κ_Q, be considered as a phenomenological quantity for which a measurement procedure has to be defined.

It is often reasonable to disregard the variation of the absorption and the scattering coefficient with temperature in the surface layer. The term containing L^{h} in Eq. (33) acts then as an external source for the temperature field depending only on the physical conditions at the boundary. This is a significant conceptual simplification and computational advantage. The problem of the combined processes of heat conduction and radiative transport reduces formally to a heat conduction problem, now with a clearly temperature dependent effective conductivity coefficient κ_{hrt}, and with a volumetric external heat source due to the solution of the homogeneous equation of radiative transfer important only in a region near the surface.

As indicated by Eq. (23), the validity of the approximations used in this section rests on smoothness assumptions for the temperature fields which are difficult to discuss in general terms since temperature is not externally given in most cases but as the solution of a differential equation. Therefore, the question arises how numerical predictions using the above scheme compare with exact solutions for realistic problems. An answer is not readily found as numerical solutions of the full equation of radiative transfer combined with the equations for heat conduction are not easily achieved. For this reason the question of the numerical reliability of the completed diffusion approximation proposed here is discussed in the framework of the two-flux model for radiative transfer.

4. Diffusion approximation and the two-flux model

If spatial variations of the physical quantities occur only in one direction x the two-flux model [9,13,14] is a valuable simplifying approximation of the full equation of radiative transfer. Here, the description of the radiative field is reduced to two radiant energy flows E_+ and E_- in the positive and the negative x-direction, the irradiances. The two-flux equations are conveniently expressed by

$$J = E_+ - E_-, \tag{36}$$

$$F = 2(E_+ + E_-) \tag{37}$$

corresponding to the quantities defined by the equations (9) and (10). J is again the net power flow of the radiation field and F is the total energy density times the local velocity of light if the radiation field is isotropic in each half space around the positive and the negative x-directions which is the basic assumption of the Milne–Eddington approximation [13,14].

With these variables, the two-flux equations can be written as

$$\frac{\mathrm{d}J}{\mathrm{d}x} = -\frac{A}{2}(F - q), \tag{38}$$

$$\frac{\mathrm{d}F}{\mathrm{d}x} = -2(A + 2S)J, \tag{39}$$

where A and S describe the absorption and scattering properties of the material. We take here A and S independent of the wavelength (gray slab). The emission term q is then given by

$$q = 4\sigma_B T(x)^4. \tag{40}$$

For a slab of thickness X, $0 \leqslant x \leqslant X$, and if the absorption and the scattering coefficient are independent of x the solution of the homogeneous equations ($q = 0$) is given by [2, 14.3]

$$J^h(x) = D_- e^{-Wx} + D_+ e^{-W(X-x)}, \tag{41}$$

$$F^h(x) = \frac{2W}{A}(D_- e^{-Wx} - D_+ e^{-W(X-x)}), \tag{42}$$

with

$$W = A\sqrt{1 + 2S/A}, \tag{43}$$

the two coefficients D_- and D_+ being given by boundary values of J^h and F^h.

An approximate solution of the Eqs. (38) and (39) is found by solving these equations for J and F and by performing an iteration process starting with $J = 0$, $F = q$. The result of the first iteration step is

$$J^i = -\frac{1}{2(A + 2S)}\frac{\mathrm{d}q}{\mathrm{d}x}, \tag{44}$$

$$F^i = q + \frac{1}{A}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{A + 2S}\frac{\mathrm{d}q}{\mathrm{d}x}\right). \tag{45}$$

These equations are identical with Eqs. (24) and (25) if one sets

$$\psi_0 = \frac{2}{A}, \tag{46}$$

$$\psi_1 = \frac{3}{2}\frac{1}{A + 2S} = \psi_1^{\mathrm{eff}}. \tag{47}$$

5. Numerical comparison of the diffusion approximation with exact solutions

In order to test the validity of the diffusion approximation we consider stationary heat conduction and radiative energy transport in a slab within the two-flux model. For a stationary process in the slab, it is

$$J_Q(x) + J_{\mathrm{rad}}(x) = J_{\mathrm{tot}} = \mathrm{const.} \tag{48}$$

where J_Q and J_{rad} are given by Eqs. (27) and (28).

As a specific example, we study a gray slab of thickness X, $0 \leqslant x \leqslant X$, with κ_Q, A, S independent of x, which is irradiated at the side $x = 0$ with the constant power density N and held at temperature $T = T_1$ at the boundary $x = X$. At $x = 0$, the slab is thermally isolated, i.e. $J_Q(0) = 0$. We further assume at the boundary X that

$$E_-(X) = \rho_1 E_+(X) + (1 - \rho_1)\sigma_B T_1^4, \tag{49}$$

i.e. the flux entering the slab at the right border is equal to the reflected part, with coefficient ρ_1, of the flux leaving the slab plus the thermally emitted flux of the thermostat.

For a gray material we have

$$J_{\mathrm{rad}} = J \tag{50}$$

and the problem is described by the following set of equations

$$\frac{\mathrm{d}T}{\mathrm{d}x} = \frac{J - J_{\mathrm{tot}}}{\kappa_Q}, \tag{51}$$

$$\frac{\mathrm{d}J}{\mathrm{d}x} = -\frac{A}{2}(F - 4\sigma_B T^4), \tag{52}$$

$$\frac{\mathrm{d}F}{\mathrm{d}x} = -2(A + 2S)J, \tag{53}$$

with the boundary conditions

$$\frac{dT}{dx}(0) = 0, \tag{54}$$

$$J(0) = J_{tot}, \tag{55}$$

$$F(0) = 4N - 2J_{tot}, \tag{56}$$

$$T(X) = T_1, \tag{57}$$

$$J(X) = \frac{\theta}{2}(F(X) - 4\sigma_B T_1^4), \tag{58}$$

with

$$\theta = \frac{1-\rho_1}{1+\rho_1}. \tag{59}$$

For the sake of a numerical solution of these equations, the variables J and F can be eliminated and the problem be formulated in the variables $T(x)$ and $J_Q(x)$ thus reducing the number of unknown functions by one. Inserting

$$J = J_{tot} + \kappa_Q \frac{dT}{dx}, \tag{60}$$

into Eq. (53) yields a differential equation that can be integrated for constant material properties and one gets with the boundary condition (56)

$$F(x) = 2\{2N - (A+2S)\kappa_Q[T(x) - T_0] - J_{tot}(1 + [A+2S]x)\}, \tag{61}$$

where

$$T_0 = T(0). \tag{62}$$

For the functions

$$\tau(x) = T(x) - T_0 \tag{63}$$

and $J_Q(x)$, the system of differential equations

$$\frac{d\tau}{dx} = -\frac{J_Q(x)}{\kappa_Q}, \tag{64}$$

$$\frac{dJ_Q}{dx} = A[2N - (A+2S)\kappa_Q\tau(x) - J_{tot}\{1 + (A+2S)x\} - 2\sigma_B\{\tau(x) + T_0\}^4] \tag{65}$$

is obtained with the boundary conditions

$$\tau(0) = 0, \tag{66}$$

$$J_Q(0) = 0, \tag{67}$$

$$\tau(X) = T_1 - T_0, \tag{68}$$

$$J_Q(X) = J_{tot} - \theta[2N - (A+2S)\kappa_Q(T_1 - T_0) - J_{tot}\{1 + (A+2S)X\} - 2\sigma_B T_1^4]. \tag{69}$$

The parameters T_0 and J_{tot} must be determined in such a way that the boundary conditions for $\tau(X)$ and $J_Q(X)$ are matched.

The following numerical example treats a shielding problem: A body at a low temperature T_1 should be protected against a high impinging radiative flux N. But the same setting also describes an insulation problem: A body at a high temperature T_1 is isolated with respect to radiative losses. The surface at $x = 0$ is then subjected only to a low radiative flux e.g. from the surroundings at ambient temperature. Note that temperature is continuous at the position $x = X$, the boundary between two material bodies in thermal contact. There is no need for jump boundary conditions [7] of temperature.

5.1. Solution with diffusion approximation

With the diffusion approximation for the gray body, the quantities J and F are approximated in lowest order by

$$J = J^h + J^i = J^h - \frac{8\sigma_B}{A+2S}T^3\frac{dT}{dx}, \tag{70}$$

$$F = F^h + F^i = F^h + 4\sigma_B T^4. \tag{71}$$

(see Eqs. (44) and (45)) where $J^h(x)$ and $F^h(x)$ are given functions depending linearly on the two parameters D_- and D_+ (see Eqs. (41) and (42)). The functions $J(x)$ and $F(x)$ are, therefore, determined by $T(x)$ and the two real numbers D_- and D_+. With the above decomposition of the radiative field, Eq. (48) can be integrated yielding

$$\int_{T(0)}^{T(x)} dT\kappa_{hrt}(T) = \int_0^x dx\prime J^h(x\prime) - xJ_{tot}, \tag{72}$$

under the condition that κ_{hrt}, given by Eqs. (35) and (47), depends only implicitly on x, i.e. only through the function $T(x)$. The left hand side accounts for the contributions of J_Q and J^i to Eq. (48). Note that for a gray body with constant material properties

$$\int_0^x dx' J^h(x') = \frac{F^h(0) - F^h(x)}{2(A+2S)}. \tag{73}$$

Using Eq. (48) and the boundary conditions (54)–(58) we get the following set of boundary conditions for the variables J^h, F^h, T

$$\frac{1}{2}F^h(0) + J^h(0) + 2\sigma_B T(0)^4 = 2N, \tag{74}$$

$$J^h(0) = J_{tot}, \tag{75}$$

$$T(X) = T_1, \tag{76}$$

$$\frac{1}{2}\theta F^h(X) - (1-\eta)J^h(X) = \eta J_{tot}, \tag{77}$$

with θ given by Eq. (59) and the constant η by

$$\eta = \frac{8\sigma_B T_1^3}{(A+2S)\kappa_Q + 8\sigma_B T_1^3} = \frac{J^i(X)}{J_Q(X) + J^i(X)} \leqslant 1. \tag{78}$$

The quantity η parametrises the quotient of the heat flow $J_Q(X)$ and of the radiative flow due to the special solution $J^i(X)$ at the border $x = X$. Eq. (77) follows from the observation that only two of the four quantities J_Q, J^i, J^h, J_{tot} can be independently chosen because of Eq. (78) and of the energy balance $J_Q(x) + J^i(x) + J^h(x) = J_{tot}$. To get Eq. (77) the quantity $J = J^i + J^h$ is expressed by a linear combination of J^h and J_{tot}.

The diffusion approximation allows for the analytical integration of all differential equations involved. Eq. (72) is the defining equation of the function $T(x)$ in terms of the four parameters D_-, D_+, $T(0)$, and J_{tot}. These parameters can be calculated from the four boundary conditions (74)–(77) and from Eq. (72) at $x = X$. The resulting set of equations is linear in D_-, D_+, J_{tot} and requires to find the root of a non-linear function to determine the surface temperature $T(0)$. The four parameters once determined, Eq. (72) gives the value of $T(x)$ as the root of a non-linear function. For this task, fast and reliable algorithms are available (see e.g. [10]).

A numerical example calculated with the diffusion approximation is represented in Fig. 1. The figure shows the temperature T, the total energy flow J_{tot} across the layer, the radiative flow J_{rad}, its contribution J^h due to the solution of the homogeneous two-flux equations, the flow quantity F that indicates the local radiative energy density, and its homogeneous part F^h. The difference between J_{tot} and J_{rad} is the heat flow J_Q, the difference between J_{rad} and J^h the contribution J^i of the diffusion approximation. A 5 mm thick layer is considered irradiated at $x = 0$ with $9.073 \times 10^5\ \mathrm{W\,m^{-2}}$ corresponding to the total irradiance of a black surface at 2000 K. The layer is kept at 300 K at the other boundary. The thermostat perfectly reflects radiation ($\rho_1 = 1.0$). The absorption coefficient of the material is $1000\ \mathrm{m^{-1}}$, the scattering coefficient equals $10612\ \mathrm{m^{-1}}$ yielding a reflection coefficient of the material of 0.65, and the coefficient of heat conduction is $0.2\ \mathrm{W\,K^{-1}\,m^{-1}}$. Rather low values for the absorption coefficient and for the coefficient of heat conduction have been chosen in this example in order to make the different contributions to the radiative field and to the total energy flow through the sample clearly visible.

The physical radiative properties of the system are given by the functions $J_{rad}(x)$ and $F(x)$ the solutions J^h and F^h being auxiliary quantities that are important only near the boundaries but are indispensable there for a coherent description. Since there is no heat flow across the hot boundary in our example the temperature gradient is zero

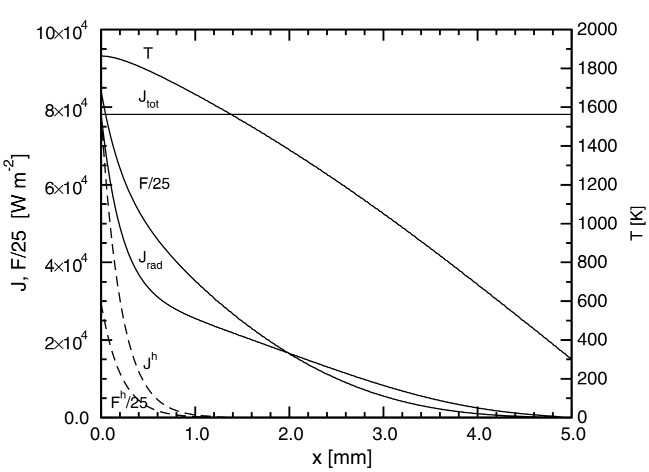

Fig. 1. Example of a numerical calculation using the diffusion approximation. All radiative quantities and the heat flow refer to the left scale, temperature to the right scale. F and F^h are rescaled with a factor 0.04 in order to get a compact diagram.

at this boundary implying that the contribution J^i of the diffusion approximation to the radiative energy flow vanishes there and the total energy flow is carried by J^h. Clearly, the diffusion approximation cannot properly account for the physical situation here if the contribution of the homogeneous two-flux equations is disregarded.

It can be seen in Fig. 1 how the heat flow J_Q is built up near the hot surface at the expense of the radiative flow J_{rad}. Near the cold surface, the quantity J^h attains a slightly negative value of $\approx -200\ \mathrm{W\,m^{-2}}$ in order to compensate for the positive value of J^i enforced by the negative temperature gradient since $J_{rad}(X)$=0. Near the hot boundary, the ratio $J^i/J_Q = 0.661$, at the cold boundary $J^i/J_Q = 2.76 \times 10^{-3}$. With the values for A and S chosen, W^{-1} equals 0.212 mm. At the position $x = 1.0$ mm, corresponding to about $4.7 \times W$, the homogeneous solution is already small compared with its initial value. The quantity F^h attains its minimal value of $0.59\ \mathrm{W\,m^{-2}}$ at $x = 3.13$ mm and rises to $2031\ \mathrm{W\,m^{-2}}$ at the cold boundary which accounts for about 2/3 of the value of F at this position.

5.2. Numerical comparison

For the sake of a numerical comparison of the exact model described by the Eqs. (51)–(59) or Eqs. (63)–(69), respectively, with the diffusion approximation described in Section 5.1, a set of material properties has been chosen that is geared to the values of semi-crystalline zirconia. The following numerical values of the material parameters and the boundary conditions are used for the computations: incident radiative flow $N = 9.073 \times 10^5\ \mathrm{W\,m^{-2}}$, temperature of thermostat $T_1 = 300$ K, reflectivity of thermostat $\rho_1 = 1.0$, coefficient of heat conduction $k_Q = 2.0\ \mathrm{W\,K^{-1}\,m^{-1}}$, scattering coefficient divided by absorption coefficient $S/A = 10.612$ corresponding to a reflection coefficient 0.65 of an infinitely thick layer. This value is the mean reflection coefficient of yttria stabilised semi-crystalline zirconia below 1800 K [15]. The incident radiative flow N corresponds to the total irradiance of a black surface at 2000 K. A typical value of the absorption coefficient for zirconia at low temperature is $A = 10^4\ \mathrm{m^{-1}}$ [16]. For the numerical study, the value of the absorption coefficient was varied keeping the quotient S/A constant and a set of five different layer thicknesses were considered covering the range of a semitransparent to a completely opaque layer: $d = 0.1$, 0.2, 1, 5 and 10 mm.

The implementation of the diffusion approximation into computer code results in a fast and reliable program that works well for every physically reasonable input. The program for the exact model amounts to find a root in the two-dimensional parameter space (T_0, J_{tot}), the boundary conditions (68) and (69) being the target functions. For given initial values of T_0 and J_{tot}, $\tau(X)$ and $J_Q(X)$ are the result of the numerical integration of the differential Eqs. (64) and (65) these equations also being dependent on T_0 and J_{tot}. All multi-dimensional root finders require sufficiently close starting values for convergence. It was found that the diffusion approximation provides such sufficiently close starting values at least for low absorption coefficients. Therefore, the following procedure was adopted to calculate the exact solution: if the diffusion approximation does not provide sufficiently close initial values of T_0 and J_{tot} for the envisaged value A_{final} of the absorption coefficient a decreasing sequence of trial A-values is chosen until the root finder converges. Starting from this value the absorption coefficient is augmented step by step the roots of the previous step always being the starting values of T_0 and J_{tot} for the next step until, hopefully, the desired value A_{final} has been reached.

However, for a given layer thickness d, it was found that there exists an upper bound A_{max} for the values of the absorption coefficient accessible in this way. This bound is given by the condition $10.0 \leqslant d \cdot W(A_{max}) \leqslant 11.5$ for the chosen physical properties and layer thicknesses. This behaviour can be explained by noting that the analytical solution of the homogeneous two-flux equations is also part of the solution of the inhomogeneous equations for a given temperature field. Integrating numerically these equations from one side implies that the solution contains an exponentially increasing part. A small change of the initial conditions or likewise numerical scatter at the start is blown up exponentially leading to a breakdown of the root finding algorithm for high values of the optical thickness of the layer. In physical terms, one may state that it is not possible to target radiative boundary conditions across an optically thick layer. This is a principal limitation of the analytic approach formulated by the Eqs. (64)–(69). In contrast, the solutions calculated with the diffusion approximation are not subjected to such restrictions.

For the numerical comparison, the relative differences of the total energy flow across the layer calculated with the exact model and with the diffusion approximation

$$\Delta J_{rel} = 1 - \frac{J_{tot}^{dif.ap.}}{J_{tot}^{exact}}, \tag{79}$$

in function of the absorption coefficient were chosen as indicators for the quantitative agreement of the two approaches (see Fig. 2). The parameter sweep starts with the rather low value $A = 10\ \mathrm{m}^{-1}$ of the absorption coefficient for every layer thickness and extends to the aforementioned upper bounds numerically accessible for the exact model. It can be seen that the relative deviations typically decrease with increasing values of the absorption coefficient A except for the two thickest layers where there is, first, a slight increase before the relative differences start to decrease. For each value of the layer thickness, the upper bound A_{max} limiting the numerical calculation of the exact solution is indicated by a sharply increasing scatter of ΔJ_{rel} if A approaches these bounds. The quantity $|\Delta J_{rel}|$ decreases roughly proportional to A^{-1} from $|\Delta J_{rel}| \approx 5 \times 10^{-2}$ at $A = 10\ \mathrm{m}^{-1}$ to $|\Delta J_{rel}| \approx 5 \times 10^{-4}$ at $A = 10^3\ \mathrm{m}^{-4}$ for the layers with 0.1, 0.2 and 1.0 mm thickness and, further, to $|\Delta J_{rel}| \approx 3 \times 10^{-5}$ at $A = 10^4\ \mathrm{m}^{-1}$ for the two

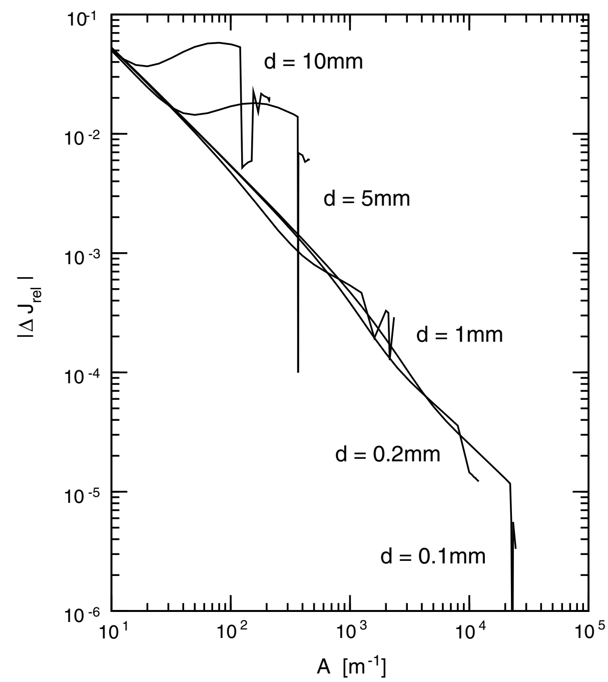

Fig. 2. Relative differences of the total heat flows calculated with the exact model and the diffusion approximation as functions of the absorption coefficient for five different layer thicknesses.

thinnest layers. For the 5 mm and the 10 mm layer, $|\Delta J_{rel}| \approx 5 \times 10^{-2}$ for $A = 10\ \mathrm{m}^{-1}$ and decreases first in both cases but increases then slightly reaching a flat maximum at $A \approx 80\ \mathrm{m}^{-1}$ and $A \approx 200\ \mathrm{m}^{-1}$ with deviations of 5% and 2%, respectively, of the diffusion approximation from the exact solution. We conclude that the diffusion approximation is reliable for the problem discussed for physically relevant values of the absorption coefficient ($A \geqslant 10^3\ \mathrm{m}^{-1}$).

The numerical comparison shows that the solution using the diffusion approximation is close to the exact solution for physically relevant values of the material parameters. The computational procedure used for the solution with the diffusion approximation reveals, further, distinct numerical advantages over the procedure for the exact problem. The same structural advantages of the diffusion approximation provide fast and reliable numerical algorithms also for time dependent heat and radiative transport problems [17].

Acknowledgements

Financial support by the Swiss Federal Office of Energy is gratefully acknowledged.

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