Application of the statistical narrow-band correlated-k method to non-grey gas radiation in CO2-H2O mixtures: approximate treatments of overlapping bands

Liu, Fengshan; Smallwood, Gregory; Gulder, O.

Publisher's version / Version de l'éditeur:
https://doi.org/10.1016/S0022-4073(00)00033-9
IEEE Acoustics, Speech, and Signal Processing Newsletter, 68, February 4, pp. 401-417, 2001

NRC Publications Record / Notice d'Archives des publications de CNRC:
https://nrc-publications.canada.ca/eng/view/object/?id=a1798a22-b68c-48e2-bf59-576b88945091
https://publications-cnrc.canada.ca/fra/voir/objet/?id=a1798a22-b68c-48e2-bf59-576b88945091

MARIA CLANCY
DGO
INST FOR CHEM PROCESS & ENVIR TECH
NATIONAL RESEARCH COUNCIL CANADA
M-12, ROOM 141, 1200 MONTREAL RD.
OTTAWA, ON K1A 0R6
CANADA

Client Number:	MARIA E. CLANCY
Title:	**JOURNAL OF QUANTITATIVE SPECTROSCOPY AND RADIATIVE TRANSFER**
Vol./Issue:	68
Date:	2001
Pages:	401-417
Article Title:	APPLICATION OF THE STATISTICAL NARROW-BAND CORRELATED-K METHOD TO NON-GREY GAS RADIATION IN CO2-H2O MIXTURES: APPROXIMATE TREATMENTS OF OVERLAPPING BANDS
Article Author:	LIU, F.; SMALLWOOD, G.J.; GULDER, O.L.

INSTRUCTIONS: NEEDED BY: 17 APRIL 2009

Estimated cost for this 17 page document: $0 document supply fee + $0 copyright = $0

PERGAMON

Journal of Quantitative Spectroscopy & Radiative Transfer 68 (2001) 401–417

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

Application of the statistical narrow-band correlated-k method to non-grey gas radiation in CO_2–H_2O mixtures: approximate treatments of overlapping bands

Fengshan Liu*, Gregory J. Smallwood, Ömer L. Gülder

Combustion Research Group, Institute for Chemical Process and Environmental Technology, National Research Council, Montreal Road, Ottawa, Ont., Canada K1A 0R6

Received 15 June 1999

Abstract

The statistical narrow-band correlated-k method was employed to calculate narrow-band intensities along a line-of-sight and radiative transfer in a three-dimensional rectangular enclosure containing nonisothermal CO_2–H_2O–N_2 mixtures at 1 atm. The correlated treatment of overlapping narrow bands of CO_2 and H_2O based on the multiplication property of gas transmissivity significantly increases the execution time of this method at each overlapping band. Three new approximate treatments for overlapping bands were proposed to improve the computational efficiency of the statistical narrow-band correlated-k method for gas radiation calculations in media containing two or more radiating gases. The accuracy of the statistical narrow-band correlated-k method using four approximate treatments of overlapping bands in CO_2–H_2O–N_2 mixtures was evaluated by comparing their numerical results with those obtained using the correlated treatment of overlapping bands. Such comparisons were made for both spectrally integrated quantities and narrow-band intensities along a line-of-sight. Results of the statistical narrow-band model were also obtained as a reference solution in the evaluation of the results of the statistical narrow-band correlated-k method.

1. Introduction

Development of accurate and efficient non-grey gas radiation models is important to many practical applications and fundamental research of flame and combustion phenomena. The recently developed spectral-line-based weighted-sum-of-grey-gases model (SLWSGG) [1,2] is by

* Corresponding author. Tel.: + 1-613-993-9470; fax: 1-613-957-7869.
E-mail address: fengshan.liu@nrc.ca (F. Liu).

0022-4073/01/$ - see front matter.
PII: S0022-4073(00)00033-9

far the best choice for calculations of total (spectrally integrated) quantities, such as wall heat fluxes and the volumetric source term, based on the considerations of accuracy and computational efficiency [3,4]. The SLWSGG model is a powerful tool for coupling gas radiation heat transfer with other processes such as fluid flow and combustion in the simulation of multi-dimensional combustion systems. While spectrally integrated quantities are of interest for radiative heat transfer, information on low-resolution spectral intensities is required in many other applications such as remote sensing and infrared detection. For these applications a narrow-band model has to be employed in order to provide the desired spectral resolution, which is generally in the range of 5–100 cm^{-1}.

Narrow-band models developed in the literature can be grouped into two types. The first type consists of all the classical narrow-band models which yield narrow-band averaged gas transmissivity. The most widely used such model is the statistical narrow-band (SNB) model [5,6]. Implementation of such classical narrow-band models into the radiative transfer equation (RTE) suffers from some major difficulties. First, the resultant transfer equation contains a correlation term which is very time-consuming to calculate [7]. Second, solution of the transfer equation requires a ray-tracing procedure which is computationally demanding in multidimensions. Third, these models are incompatible with radiation scattering, although this difficulty can be alleviated to some extent by using the variable splitting strategy suggested by Liu et al. [8]. Due to these difficulties, the classical narrow-band models are not widely used.

Models of the second type are those based on the concept of the weighted-sum-of-grey-gases (WSGG) first proposed by Hottel and Sarofim [9], such as the narrow-band weighted-sum-of-grey-gases (NBWSGG) model developed by Yang and Song [10] and various correlated-k (CK) models. Correlated-k models can be formulated either by analysing the HITRAN database, by fitting the narrow-band averaged gas transmissivity to some empirical expressions [6], or by inverse Laplace transformation of the gas transmissivity based on a classical narrow-band model [11]. WSGG-based narrow-band models provide information about the gas absorption coefficient and therefore enjoy the advantage that the accurate and efficient discrete-ordinates method (DOM) can be used to solve the transfer equation. In addition, effect of radiation scattering can be accounted for easily in these models.

The statistical narrow-band correlated-k (SNBCK) model described by Lacis and Oinas [11] is not new to atmospherical transfer, but is a relatively new concept to the radiative heat transfer community. This method has been recently used to calculate real-gas radiation in a two-dimensional rectangular enclosure by Goutière et al. [4]. The SNBCK method offers two advantages compared to other CK methods. Firstly, the cumulative distribution function is expressed analytically as a function of the absorption coefficient and its inversion can be achieved very efficiently using a Newton–Raphson procedure. Secondly, the effect of pressure is formulated into the model through the SNB gas transmissivity expression. This is in contrast to the CK method of Soufiani and Taine [6] where the model parameters are pre-calculated for a given pressure. In addition, the SNBCK is also an ideal candidate for prediction of low-resolution spectral intensity.

Despite the advantages of CK methods mentioned above, these models encounter some difficulty at overlapping bands, which occurs when these models are applied to gas radiation transfer in media containing more than one radiating gas, such as CO_2 and H_2O. It is worth noting that almost all practical problems involve two or more radiating gases. The most generally accepted approach to overlapping bands is to apply the multiplication property of gas transmissivity [11].

As a result, the computational efforts of a WSGG-based narrow-band model at an overlapping band increase by a factor of N (N is the number of quadrature points) for each additional radiating gas.

In order to improve the computational efficiency of the SNBCK method at overlapping bands, three approximate treatments were developed in the present study. The accuracy of these approximate treatments and another approximate method proposed by Lacis and Oinas [11] was evaluated for both narrow-band intensities along a-line-of-sight and for spectrally integrated quantities in a three-dimensional rectangular enclosure containing CO_2–H_2O–N_2 mixtures at 1 atm.

2. Formulation

The SNBCK method has been described in detail by Lacis and Oinas [11] and also by Goody et al. [12]. Only a brief outline of this method is given below to assist the discussion of overlapping band treatments.

The starting point of CK methods is that for any radiative quantity ϕ_ν that is solely dependent on gas absorption coefficient (this is true for a narrow-band where the blackbody function can be treated as a constant) the integration over wavenumber can be replaced by integration over the absorption coefficient

$$\bar{\phi}_\nu = \frac{1}{\Delta\nu}\int_{\Delta\nu}\phi(\kappa_\nu)\,\mathrm{d}\nu = \int_0^\infty f(k)\phi(k)\,\mathrm{d}k, \tag{1}$$

where

$$f(k) = \frac{1}{\Delta\nu}\frac{\mathrm{d}\nu}{\mathrm{d}k} \tag{2}$$

is the normalised distribution function of the gas absorption coefficient inside $\Delta\nu$ and $f(k)\,\mathrm{d}k$ represents the fraction of wavenumber inside $\Delta\nu$ where the gas absorption coefficient lies between k and $k + \mathrm{d}k$. Note that when the integration over wavenumber is replaced by integration over the gas absorption coefficient, the spectral gas absorption coefficient κ_ν is denoted by k since it now plays the role of an independent variable and is no longer a function of wavenumber. Application of Eq. (1) to gas transmissivity leads to

$$\bar{\tau}_\nu(L) = \int_0^\infty f(k)\exp(-kL)\,\mathrm{d}k. \tag{3}$$

Determination of the distribution function $f(k)$ can be achieved through two ways. One is to analyse the HITRAN database as has been conducted by Tang and Brewster [13]. The other is to perform the inverse Laplace transformation of the gas transmissivity of a narrow-band model based on Eq. (3) as in the SNBCK method described by Lacis and Oinas [11].

In the SNB model, the gas transmissivity over an isothermal and homogeneous path is given as [5]

$$\bar{\tau}_\nu(L) = \exp\left[-\frac{\pi B}{2}\left(\sqrt{1+\frac{4SL}{\pi B}}-1\right)\right], \tag{4}$$

where $B = 2\bar{\beta}_v/\pi$, $S = \bar{k}_v fp$, L is the path length, f the mole fraction of the radiating gas, p the pressure, and $\bar{\beta}_v = 2\pi\bar{\gamma}_v/\bar{\delta}_v$ the average line width to spacing ratio. The updated SNB model parameters due to Soufiani and Taine [6], i.e. $\bar{\gamma}_v$, $\bar{\delta}_v$, and $\bar{k}_v$, for CO_2 and H_2O over a wide range of temperature were used in the present calculations. The bandwidth is uniform at 25 cm^{-1} and the covered spectral range is 150–9300 cm^{-1}. The analytical expression of $f(k)$ obtained by inverse Laplace transformation of the SNB gas transmissivity given in Eq. (4) is written as [11,14]

$$f(k) = \frac{1}{2}k^{-3/2}(BS)^{1/2}\exp\left[\frac{\pi B}{4}\left(2 - \frac{S}{k} - \frac{k}{S}\right)\right]. \tag{5}$$

The cumulative function $g(k)$ is defined as

$$g(k) = \int_0^k f(k')\,\mathrm{d}k' \tag{6}$$

which is a monotonically increasing function from 0 to 1. Using Eqs. (5) and (6), the analytical expression of $g(k)$ has been derived by Lacis and Oinas [11]

$$g(k) = \frac{1}{2}\left[1 - \mathrm{erf}\left(\frac{a}{\sqrt{k}} - b\sqrt{k}\right)\right] + \frac{1}{2}\left[1 - \mathrm{erf}\left(\frac{a}{\sqrt{k}} + b\sqrt{k}\right)\right]\mathrm{e}^{\pi B}, \tag{7}$$

where $a = \frac{1}{2}\sqrt{\pi BS}$, $b = \frac{1}{2}\sqrt{\pi B/S}$, and $\mathrm{erf}(x)$ is the error function given as

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \mathrm{e}^{-t^2}\,\mathrm{d}t. \tag{8}$$

Using the cumulative function g, the narrow-band average of any radiative variable dependent solely on the gas absorption coefficient ϕ_v can be calculated as

$$\bar{\phi}_v = \frac{1}{\Delta v}\int_{\Delta v}\phi(\kappa_v)\,\mathrm{d}v = \int_0^1 \phi(g)\,\mathrm{d}g. \tag{9}$$

Eq. (9) can be conveniently calculated using a Gauss quadrature scheme

$$\bar{\phi}_v = \sum_{i=1}^{N} w_i\phi(g_i), \tag{10}$$

where N is the number of quadrature points or grey gases used in the evaluation. Good accuracy is achieved using about 10 quadrature points [11,12]. The 7-point Gauss–Labatto quadrature has been by far the most popular one based on the considerations of accuracy and computer time [6,10,15]. It is therefore also used in the present calculations. Table 1 lists the weight parameters, w_i, and the quadrature point g_i of the 7-point Gauss–Labatto scheme.

In the calculation of the SNBCK method, a radiative quantity at the ith quadrature point, $\phi(g_i)$, is actually obtained in terms of its corresponding absorption coefficient, i.e. $\phi(k_i)$, since the RTE is formulated in such a way that the absorption coefficient appears as the radiative property. The absorption coefficient k_i corresponding to the ith quadrature point g_i is obtained by inversion of the cumulative distribution function given in Eq. (7). Although an analytical expression for $k(g_i)$ does not exist, it can be found numerically by using a Newton–Raphson iteration method with only

Table 1
The 7-point Gauss–Labatto quadrature scheme

i	g_i	w_i
1	0.00000	0.04500
2	0.15541	0.24500
3	0.45000	0.32000
4	0.74459	0.24500
5	0.90000	0.05611
6	0.93551	0.05125
7	0.98449	0.03764

a few iterations when k_{max} (where $f(k)$ peaks) is used as the initial value of k, as suggested by Lacis and Oinas [11].

For radiative transfer in three-dimensional rectangular enclosures, the transfer equation solved in the SNBCK method at each narrow band is written as

$$\xi\frac{\partial I_i}{\partial x}+\mu\frac{\partial I_i}{\partial y}+\eta\frac{\partial I_i}{\partial z}=-k_iI_i+k_iI_b \quad i=1,2,\ldots,7. \tag{11}$$

The band-averaged radiation intensity is then calculated as

$$\bar{I}=\sum_{i=1}^{7}I_iw_i. \tag{12}$$

Spectrally integrated quantities are calculated by adding the appropriate narrow-band quantities (wall heat fluxes and volumetric source term) over all the narrow bands.

For calculations of narrow-band intensities along a line-of-sight, the following recursive equation is solved:

$$\begin{aligned}I_{i,j+1}&=I_{i,j}\exp[-k_{i,j+1/2}(s_{j+1}-s_j)]\\&\quad+I_{b,j+1/2}(1-\exp[-k_{i,j+1/2}(s_{j+1}-s_j)]),\end{aligned} \tag{13}$$

where subscript j denotes spatial discretisation index and s is the spatial location along the line-of-sight under consideration.

3. Treatments of overlapping bands

The distribution function $f(k)$ given in Eq. (5) is obtained by inverse Laplace transformation of the SNB gas transmissivity which is valid only for non-overlapping bands. When dealing with gas radiation in a mixture containing two or more radiating gases (for most practical problems, these are CO_2 and H_2O), there exist a number of overlapping narrow bands at which both gases absorb and emit radiation and Eq. (5) is no longer valid. This is simply because the product of two Malkmus bands is not a Malkmus band [12]. Several methods for handling overlapping bands within the context of the SNBCK method are discussed below.

3.1. The correlated method

At an overlapping band (hereafter we consider an overlapping band of CO_2 and H_2O, but the methods described are applicable to other gases), the total gas transmissivity obeys the multiplication property, i.e.

$$\tau_{\mathrm{mix}}(L) = \tau_c(L) \times \tau_h(L)$$
$$= \exp\left[-\frac{\pi B_c}{2}\left(\sqrt{1+\frac{4S_cL}{\pi B_c}} - 1\right)\right] \times \exp\left[-\frac{\pi B_h}{2}\left(\sqrt{1+\frac{4S_hL}{\pi B_h}} - 1\right)\right], \tag{14}$$

where subscripts mix stands for mixture, c for CO_2, and h for H_2O. In this case, the distribution function of the mixture $f(k)$ is the inverse Laplace transformation of $\tau_{\mathrm{mix}}(L)$ which has no analytical solution. The correlated treatment of an overlapping band consists of the following steps. Firstly, the cumulative distribution function, Eq. (7), is used inversely to get the absorption coefficients of each gas component, k_{ci} and k_{hj}. Secondly, the transmissivity contributed by each component is calculated approximately as

$$\tau_c(L) = \sum_{i=1}^{7} w_i \exp(-k_{ci}L), \tag{15}$$

$$\tau_h(L) = \sum_{j=1}^{7} w_j \exp(-k_{hj}L). \tag{16}$$

Therefore, the transmissivity of the mixture is obtained as, based on the multiplication property,

$$\tau_{\mathrm{mix}}(L) = \left(\sum_{i=1}^{7} w_i \exp(-k_{ci}L)\right)\left(\sum_{j=1}^{7} w_j \exp(-k_{hj}L)\right)$$
$$= \sum_{i=1}^{7}\sum_{j=1}^{7} w_i w_j \exp[-(k_{ci}+k_{hj})L]. \tag{17}$$

This implies that RTE at an overlapping band takes the following form:

$$\xi\frac{\partial I_{ij}}{\partial x} + \mu\frac{\partial I_{ij}}{\partial y} + \eta\frac{\partial I_{ij}}{\partial z} = -(k_{ci}+k_{hj})I_{ij} + (k_{ci}+k_{hj})I_b$$
$$i = 1,2,\ldots,7;\ j = 1,2,\ldots,7. \tag{18}$$

The band-averaged radiation intensity is then calculated as

$$\bar{I} = \sum_{i=1}^{7}\sum_{j=1}^{7} w_i w_j I_{ij}. \tag{19}$$

Therefore, the RTE has to be solved $N \times N$ times, i.e. 7×7 in this study, at each overlapping band. For a mixture of CO_2 and H_2O, there are 96 overlapping narrow bands in the SNB database. Even for non-scattering problems, the SNB-CK with this correlated treatment of overlapping bands is quite computationally demanding. For three-dimensional problems involving radiation scattering, the SNBCK method becomes intolerably slow at overlapping bands. It is therefore necessary to

develop approximate methods for overlapping band calculations to improve the efficiency of the SNBCK method at overlapping bands.

3.2. The uncorrelated method

In the uncorrelated method, it is assumed that at each overlapping band CO_2 and H_2O have the same shape of absorption coefficient distribution, but their magnitude can be different. Therefore, the total absorption coefficient at the ith quadrature point is simply the sum of k_{ci} and k_{hi}, i.e.

$$\tau_{\mathrm{mix}}(L) = \sum_{i=1}^{7} w_i \exp[-(k_{ci} + k_{hi})L]. \tag{20}$$

As a result, the following RTE is solved at each overlapping band:

$$\xi \frac{\partial I_i}{\partial x} + \mu \frac{\partial I_i}{\partial y} + \eta \frac{\partial I_i}{\partial z} = -(k_{ci} + k_{hi})I_i + (k_{ci} + k_{hi})I_b, \quad i = 1, 2, \ldots, 7. \tag{21}$$

The band-averaged radiation intensity is then calculated as

$$\bar{I} = \sum_{i=1}^{7} w_i I_i. \tag{22}$$

3.3. Approximate Malkmus band methods

Another strategy to develop approximate treatments of overlapping bands is to assume that the product of two Malkmus bands is an approximate Malkmus band, i.e.

$$B_c\left(\sqrt{1 + \frac{4S_cL}{\pi B_c}} - 1\right) + B_h\left(\sqrt{1 + \frac{4S_hL}{\pi B_h}} - 1\right) = B_m\left(\sqrt{1 + \frac{4S_mL}{\pi B_m}} - 1\right), \tag{23}$$

where B_m and S_m are the parameters of the approximate Malkmus band for an overlapping band. The objective of formulating an approximate Malkmus band is to obtain the two parameters B_m and S_m. Once these two parameters are available, the overlapping band is treated as a non-overlapping band and the procedure described in Section 2 to calculate the absorption coefficient and intensity is followed. Three approximate Malkmus band methods are discussed below.

3.3.1. The method of Lacis and Oinas

Lacis and Oinas [11] suggested that the approximate Malkmus band parameters are calculated based on the optically thin and thick conditions. In the optically thin limit, the SNB gas transmissivity, Eq. (4), becomes

$$\bar{\tau}_v(L) = \exp(-SL). \tag{24}$$

In deriving the above expression, the approximate calculation of the square root $\sqrt{1+x} \approx 1 + \frac{1}{2}x$ is used. While in the optically thick limit, the SNB gas transmissivity approaches

$$\bar{\tau}_v(L) = \exp(-\sqrt{\pi BSL}). \tag{25}$$

The following two equations are therefore obtained for the calculation of S_m and B_m:

$$S_m = S_c + S_h, \tag{26}$$

$$\sqrt{B_m S_m} = \sqrt{B_c S_c} + \sqrt{B_h S_h}. \tag{27}$$

3.3.2. The method based on the optically thin limit

Actually, the approximate Malkmus band parameters can be derived from the optically thin condition alone using the second-order approximation $\sqrt{1+x} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2$. Application of this approximation to Eq. (23) leads to

$$S_m = S_c + S_h, \tag{28}$$

$$\frac{S_m^2}{B_m} = \frac{S_c^2}{B_c} + \frac{S_h^2}{B_h}. \tag{29}$$

3.3.3. Least-squares fitting method

The starting point of the least-squares fitting method is Eq. (23). In this method, the band model parameters B_m and S_m are obtained by minimising the error function defined below:

$$E(B_m, S_m) = \sum_{k=1}^{K} (y_k - f_k)^2, \tag{30}$$

where

$$y_k = B_m\left(\sqrt{1 + \frac{4S_m L_k}{\pi B_m}} - 1\right), \tag{31}$$

$$f_k = B_c\left(\sqrt{1 + \frac{4S_c L_k}{\pi B_c}} - 1\right) + B_h\left(\sqrt{1 + \frac{4S_h L_k}{\pi B_h}} - 1\right) \tag{32}$$

and L_k $(k = 1, 2, \ldots, K)$ is an array of path length over which the error function $E(B_m, S_m)$ is minimised. Minimisation of $E(B_m, S_m)$ requires

$$\frac{\partial E}{\partial B_m} = 0, \tag{33}$$

$$\frac{\partial E}{\partial S_m} = 0. \tag{34}$$

The above two equations are solved simultaneously using a Gauss–Siedel iteration method over a path-length range comparable to the characteristic mean path length of the problem to be solved. It is clear that this method requires more computer time to obtain B_m and S_m than the three approximate methods discussed earlier. The convergence criterion employed to stop the calculation of B_m and S_m is that the relative error of both B_m and S_m is less than 1%. Numerical experiments indicate that use of a more stringent convergence criterion significantly increases the computing time but does not further improve the accuracy of this method.

Table 2
Five treatments of overlapping narrow-bands

Method	Equations
Correlated	Eqs. (17), (18), (19)
Uncorrelated	Eqs. (20), (21)
Lacis and Oinas	Eqs. (26), (27)
Optically thin	Eqs. (28), (29)
LSF	Eqs. (33), (34)

4. Results and discussion

To test the accuracy and computational efficiency of various treatments of overlapping bands within the context of the SNBCK method, numerical calculations were conducted for both narrow-band intensities along a line-of-sight and for spectrally integrated quantities in a three-dimensional rectangular enclosure containing CO_2–H_2O–N_2 mixtures. For calculating narrow-band intensities along a line-of-sight, the emphasis is on the accuracy of different treatments of overlapping bands. The purpose of performing three-dimensional calculations are to illustrate both accuracy and efficiency of these methods.

To assist the discussions of numerical results, the five treatments of overlapping bands described in the last section are, respectively, named the *correlated*, the *uncorrelated*, *Lacis and Oinas*, *optically thin*, and least-squares fitting (LSF) method. Table 2 summarises these five methods for calculations of overlapping bands.

4.1. Narrow-band intensities along a line-of-sight

Calculations of narrow-band intensities along a line-of-sight were conducted for two cases using the SNBCK method with the five treatments of overlapping bands summarised in Table 2 to evaluate their accuracy. Narrow-band intensities were also obtained using the SNB model in order to evaluate the accuracy of the SNBCK method using the correlated treatment for overlapping bands since results of the correlated treatment are to be used as the benchmark solution in the evaluation of the other four approximate treatments of overlapping bands.

For both cases, the pressure of the gas mixture is at 1 atm and the left boundary of the gas column between $x = 0$ and 8 m is cold at 300 K and black. Narrow-band integrated intensities at $x = 8$ m along the positive x-direction were calculated by solving Eq. (13). A uniform grid of 80 was used in the calculations. In the first case, the gas mixture consists of 30% CO_2, 30% H_2O, and 40% N_2 (mole basis) and is isothermal at 1800 K. In the second case, the gas is a mixture of 10% CO_2, 20% H_2O, and 70% N_2 (mole basis) and is nonisothermal with the temperature specified as

$$T(x) = 400 + 2000\frac{x}{x_*} \quad \text{for } x < x_*$$

$$= 800 + 1600\frac{L - x}{L - x_*} \quad \text{for } x > x_*, \tag{35}$$

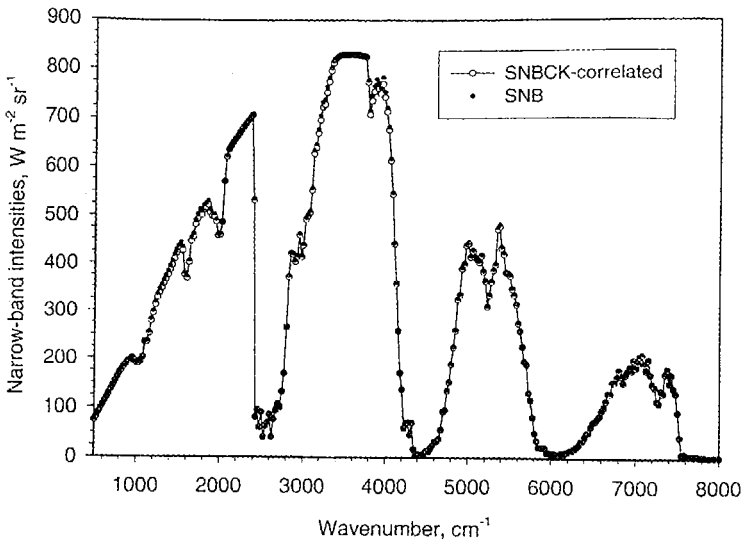

Fig. 1. Narrow-band intensities along the isothermal path obtained using the SNB model and the SNBCK-correlated method.

where $L = 8$ m and $x_* = 1.5$ m. In the calculation of the non-isothermal case using the SNB model, the Curtis–Godson approximation was used. For a mixture of CO_2 and H_2O, there are four overlapping spectral regions: 450–1200 cm^{-1} (31 bands), 1950–2450 cm^{-1} (21 bands), 3300–3800 cm^{-1} (21 bands), and 4700–5250 cm^{-1} (23 bands). Eq. (30) was fitted to a path-length range of 0–10 m using 500 non-uniform points.

Fig. 1 compares the narrow-band intensities calculated using the SNB model and the SNBCK-correlated method for the isothermal case in the wavenumber range between 500 and 8000 cm^{-1}. Hereafter, the term *SNBCK-correlated* method denotes the SNBCK method with the correlated treatment of overlapping bands and similar acronyms will be used such as *SNBCK-uncorrelated* and *SNBCK-optically thin*. Results of the SNB model and the SNBCK-correlated method are seen to be in excellent agreement for this isothermal case at most of the narrow bands. Some discrepancies between the results of these methods occur around 3700 cm^{-1} spectral region. The discrepancy between the results of these two methods in this case is attributed to quadrature errors of the SNBCK method using the 7-point Gauss–Labatto quadrature. Nevertheless, the agreement between the results of these two methods is very good and the use of the SNBCK-correlated results as the benchmark solution in the evaluation of other four approximate treatments is justified.

Narrow-band intensities calculated using the SNBCK method using the five treatments of overlapping bands are compared in Fig. 2 for the isothermal case. Results of the SNBCK-correlated method serve as the benchmark solution based on the results shown in Fig. 1. Another reason to employ the SNBCK-correlated results, instead of the SNB results, as the benchmark solution in the evaluation is that the comparison is not contaminated by quadrature errors. Except the Lacis and Oinas method, all the other three approximate treatments of overlapping bands yield narrow-band intensities in very good agreement with that of the benchmark solution, with the

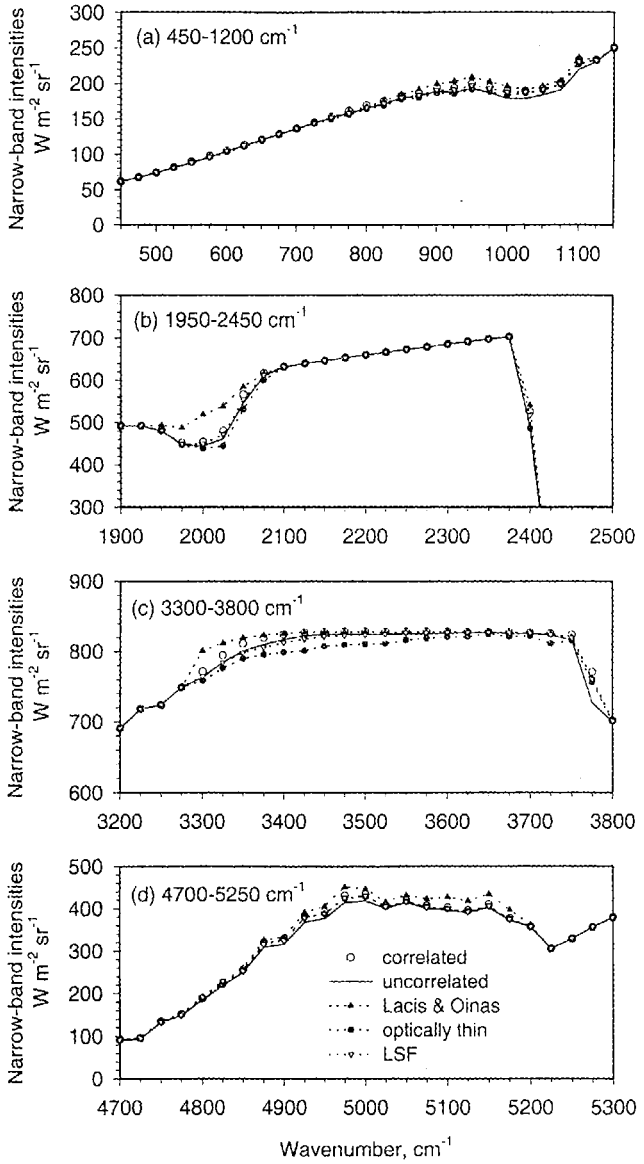

Fig. 2. Narrow-band intensities along the isothermal path obtained using the SNBCK method with the five treatments of overlapping bands for the four overlapping spectral regions: (a) 450–1200 cm^{-1}, (b) 1950–2450 cm^{-1}, (c) 3300–3800 cm^{-1}, and (d) 4700–5250 cm^{-1}.

results of the optically thin treatment less accurate at the 3300–3800 cm^{-1} overlapping spectral region. The SNBCK–Lacis and Oinas method results in significant errors at overlapping bands around 2000 and 3300 cm^{-1} spectral regions. The LSF method is the most accurate treatment of overlapping bands among the four approximate ones. In general, results of the SNBCK-uncorrelated method are very close to those of the SNBCK–LSF method.

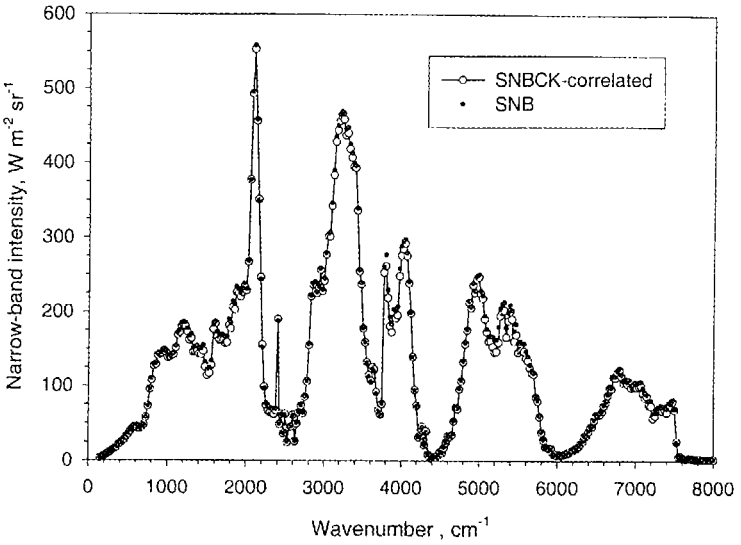

Fig. 3. Narrow-band intensities along the nonisothermal path obtained using the SNB model and the SNBCK-correlated method.

Narrow-band intensities obtained by the SNB model and the SNBCK-correlated method for the nonisothermal path are compared in Fig. 3. For calculations of radiation transfer in nonisothermal or inhomogeneous media, the Curtis–Godson approximation is often used in the SNB model to obtain equivalent model parameters, and it was also used in the present SNB calculation. The basis of the SNBCK method for such calculations is the scaling approximation [14,15]. Although these two methods make use of totally different assumptions for calculations along a non-isothermal path, good agreement is observed from the results shown in Fig. 3. Actually, the results of these two method are in very good agreement at most of the narrow bands. Except for quadrature errors in the SNBCK results demonstrated in Fig. 1, the discrepancy between the results of the SNB model and the SNBCK-correlated method observed in Fig. 3 may be largely attributed to the Curtis–Godson approximation used in the SNB model [15]. Evaluation of the accuracy of the SNB model and the SNBCK-correlated method for calculations of radiative transfer in non-isothermal media require line-by-line solutions. Such an evaluation is beyond the scope of the present study. The good agreement between the results of the SNB model and the SNBCK-correlated method found in Fig. 3 provides confidence in using the SNBCK-correlated results as benchmark solution to assess the accuracy of the other four approximate treatments of overlapping bands for this non-isothermal case.

Fig. 4 compares the narrow-band intensities calculated using the SNBCK method using the five treatments of overlapping bands for the nonisothermal path. The SNBCK-correlated results are used as the benchmark solution in the evaluation. Similar to the isothermal case, Fig. 2, the Lacis and Oinas method yields least accurate results among the four approximate methods. The other three methods, i.e. the uncorrelated, the optically thin, and the LSF, predict narrow-band intensities in good agreement with each other and with the correlated method, except in the

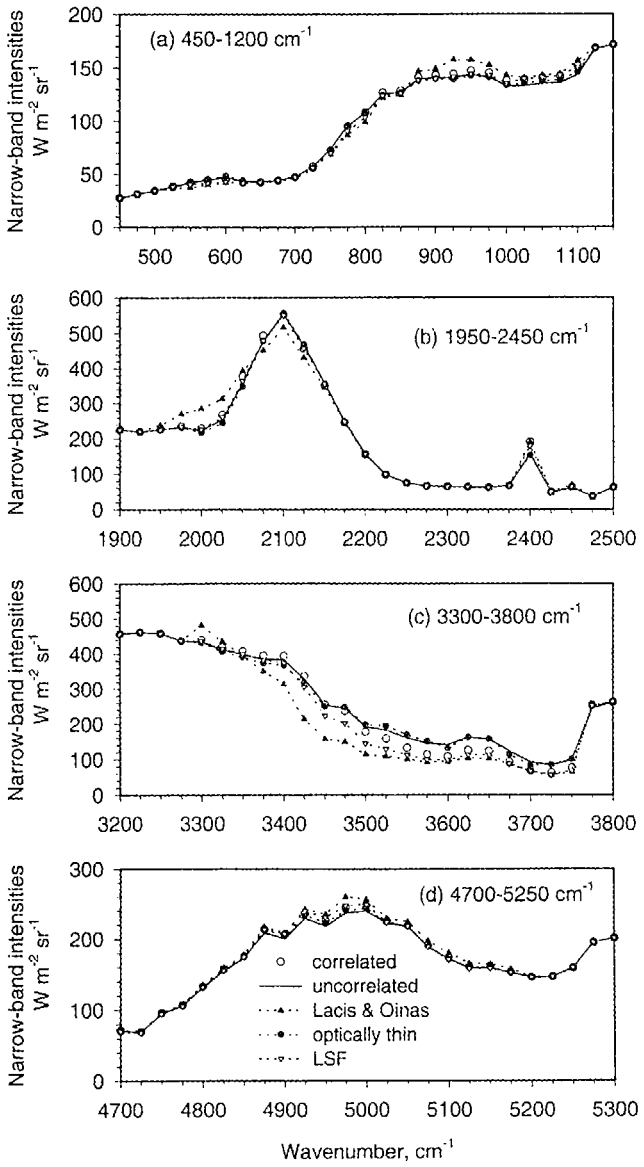

Fig. 4. Narrow-band intensities along the non-isothermal path obtained using the SNBCK method with the five treatments of overlapping bands for the four overlapping spectral regions: (a) 450–1200 cm^{-1}, (b) 1950–2450 cm^{-1}, (c) 3300–3800 cm^{-1}, and (d) 4700–5250 cm^{-1}.

3300–3800 cm^{-1} overlapping spectral region, Fig. 4(c), where all these three approximate methods yield narrow-band intensities in relatively large errors. At this overlapping spectral region, the LSF method yields the best results, although not very satisfactory at narrow bands around 3500 cm^{-1}, among the four approximate treatments of overlapping bands. It is also interesting to notice that results of the optically thin and the uncorrelated methods are very similar in this case at all four overlapping spectral regions.

4.2. Spectrally integrated quantities in a three-dimensional rectangular enclosure

The geometry of this test problem is a rectangular enclosure of 2 m × 2 m × 4 m. All the surrounding walls are black and cold at 300 K. The pressure of the gas mixture in the enclosure is kept at 1 atm. The radiating gas is a uniform mixture of 10% CO_2, 20% H_2O and 70% N_2 (mole basis). The gas temperature is non-uniform but symmetrical about the centreline of the enclosure and is specified in terms of $T = (T_c - T_e)f(r/R) + T_e$. In this equation, T_c is the gas temperature along the centreline of the enclosure, T_e is the exit temperature at $z = 4$ m. Inside the circular region of the cross section of the enclosure, the variation of gas temperature is defined by $f(r/R) = 1 - 3(r/R)^2 + 2(r/R)^3$, where r is the distance from the enclosure centreline and R is the radius of the circular region ($R = 1$ m). The gas temperature outside the circular region is assumed to be uniform and at the value of the exit temperature. The centreline temperature is assumed to increase linearly from 400 K at the inlet ($z = 0$) to 1800 K at $z = 0.375$ m, then decreases linearly to 800 K at the exit.

The RTE associated with the SNBCK method was solved using DOM. The spatial discretisation was achieved using the positive scheme and the T_4 quadrature set was used for angular discretisation which contains 128 directions in three dimensions. The enclosure was divided into 17 × 17 × 24 control volumes. A uniform grid was used in the x- and y-direction and a non-uniform grid was used in the z-direction. For this test problem, numerical results of wall heat flux and volumetric source term have been previously obtained by Liu [16] using the SNB model along with a ray-tracing algorithm and were used as a reference solution in the present evaluation.

Based on the numerical results shown in Figs. 2 and 4, it was found that the uncorrelated and the optically thin treatments of overlapping bands in general perform quite well except at overlapping narrow bands where both CO_2 and H_2O strongly absorb and emit. Therefore, in the calculations of spectrally integrated quantities in this case the LSF treatment was used only at the following overlapping bands: 600–1000, 2000–2150, and 3300–3750 cm^{-1}. For overlapping bands not in the above list, the optically thin treatment was employed.

Distributions of wall heat flux along the length of the enclosure at (2 m, 1 m, z) calculated using the SNBCK method and the five treatments of overlapping bands are compared in Fig. 5. Fig. 6 shows the volumetric source term distributions along the centreline of the enclosure, (1 m, 1 m, z). Results of the SNB model are also plotted as a reference. Although results of the SNBCK-correlated method are about 3% higher than those of the SNB model at the peak heat flux, Fig. 5, and about 4% lower at the minimum source term, Fig. 6, these discrepancies do not necessarily reflect the difference between the SNB model and the SNBCK method as a gas radiative property model in this test case since two different solvers were used. The difference between the results of the SNB model and the SNBCK-correlated method can be attributed to two factors. First, the Curtis–Godson approximation was used in the SNB model and the scaling approximation was made in the SNBCK method for calculations in non-isothermal media. In addition, some quadrature errors exist in the SNBCK-correlated method. The discrepancy due to these factors are believed to be relatively small for spectrally integrated quantities based on the results shown in Figs. 1 and 3, where the same solver was used for both the SNB model and the SNBCK method. Secondly, a ray-tracing algorithm was used to solve the transfer equation of the SNB model while the transfer equation of the SNBCK method was solved using DOM. It is well known that the numerical results of DOM using conventional spatial differencing schemes (the positive scheme

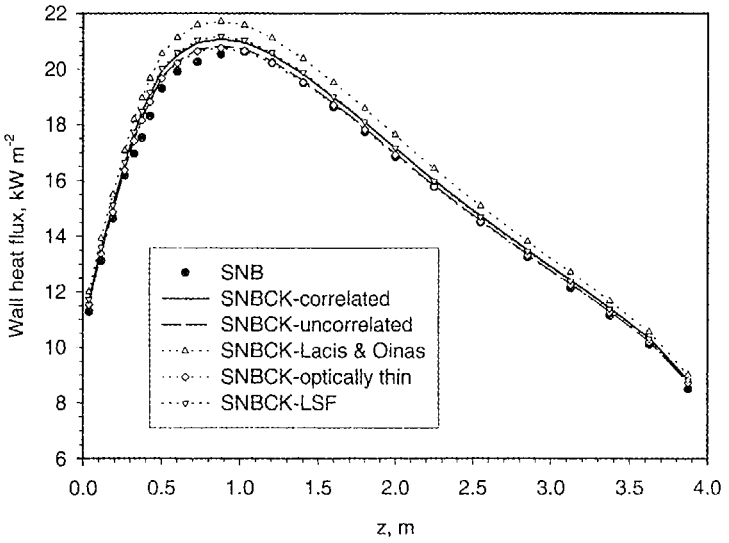

Fig. 5. Distributions of wall heat flux along the length of the enclosure at (2 m, 1 m, z) calculated using the SNB model and the SNBCK method with the five treatments of overlapping bands.

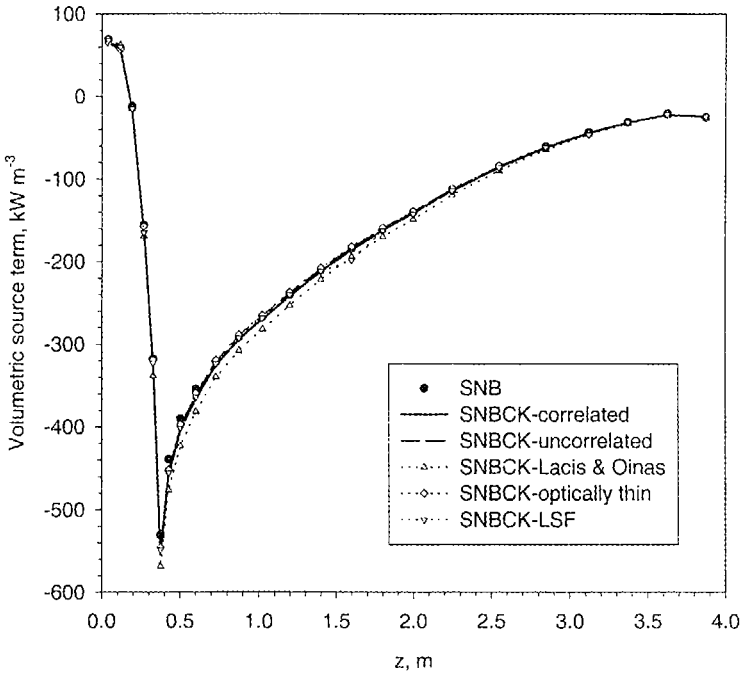

Fig. 6. Distributions of radiative source term along the centreline of the enclosure at (1 m, 1 m, z) calculated using the SNB model and the SNBCK method with the five treatments of overlapping bands.

Table 3
Comparison of CPU times for calculations of the 3D case using the SNBCK method on a SGI Octane 175 MHz

Method	CPU (s)
Correlated	25745
Uncorrelated	11862
Lacis and Oinas	11630
Optically thin	11407
LSF	11978

used here is one of them) are not very accurate in multidimensions [17]. On the other hand, a ray-tracing method offers better numerical accuracy, albeit time consuming to execute in three dimensions, since the transfer equation is solved along a line-of-sight which is one dimensional. Therefore, the numerical inaccuracy of DOM could be largely responsible for the discrepancy between the results of the SNB model and the SNBCK-correlated method found in Figs. 5 and 6. In the following discussions, results of the SNBCK-correlated method are used as the benchmark solution.

Consistent with the observations made from the results shown in Figs. 2 and 4, the Lacis and Oinas method yields the least accurate results among the four approximate treatments of overlapping bands for both the wall heat flux (Fig. 5) and the source term (Fig. 6). Results of the SNBCK–Lacis and Oinas method are in about 3% error for both wall heat flux and the centreline source term, compared to the SNBCK-correlated result. Results of the other three approximate methods, i.e. the uncorrelated, the optically thin, and LSF, are in very good agreement with those of the SNBCK-correlated method with errors less than 1%. For this test case, the SNBCK–LSF method yields spectrally integrated quantities in excellent agreement with those of the SNBCK-correlated method. Results of the SNBCK-optically thin and the SNBCK-uncorrelated methods are very close to each other.

CPU times of the SNBCK method using the five treatments of overlapping bands are compared in Table 3. The four approximate treatments of overlapping bands require very similar CPU time to execute. The correlated treatment requires a CPU time that is about a factor of 2.2 of that of an approximate treatment. This is actually expected for SNBCK calculations in CO_2–H_2O–N_2 mixtures using the 7-point Gauss–Labatto quadrature. Using the correlated treatment of overlapping bands, the CPU time is about $t_c = 271Nt + 96N^2t$, where t is the CPU time for calculations of each quadrature point. When an approximate treatment of overlapping band is used, the CPU time is about $t_a = 367Nt$. Therefore, the ratio of t_c to t_a is about $1 + 96(N - 1)/367$ which is 2.57 for $N = 7$.

5. Conclusions

Three approximate treatments of overlapping bands were developed to improve the computational efficiency of the statistical narrow-band correlated-k method at overlapping bands. The

accuracy of these three methods and the method proposed by Lacis and Oinas was evaluated against the results of the correlated treatment of overlapping bands for narrow-band intensities and spectrally integrated quantities in CO_2–H_2O–N_2 mixtures. The following conclusions are reached based on the results of the present study:

1. When overlapping bands are treated using the correlated method, the SNBCK method yields narrow-band intensities in good agreement with those of the SNB model.
2. Use of an approximate treatment of overlapping band reduces the computing time of the SNBCK method by a factor of N at an overlapping band and by more than 50% for calculations of spectrally integrated quantities in CO_2–H_2O–N_2 mixtures.
3. The overlapping band method due to Lacis and Oinas produces significant errors for narrow-band intensities along a line-of-sight and relatively small errors for spectrally integrated quantities.
4. The three approximate methods developed in this study yield accurate narrow-band intensities in the spectral regions of 450–1200, 1950–2450, and 4700–5250 cm^{-1} along an isothermal or a non-isothermal path. They predict reasonably good but not completely satisfactory narrow-band intensities in the 3300–3800 cm^{-1} overlapping spectral region. The least-squares fitting method is the most accurate treatment of overlapping bands among the four approximate ones.
5. Using the three approximate treatments of overlapping bands developed in this study, the SNBCK method yields very accurate spectrally integrated quantities. The optically thin and the uncorrelated methods are recommended for calculations of spectrally integrated quantities based on their accuracy and simplicity.

References

[1] Denison M, Webb B. J Heat Transfer 1993;115:1004.
[2] Denison M, Webb B. J Heat Transfer 1995;117:359.
[3] Bedir H, T'ien JS, Lee HS. Combustion theory and modelling, vol. 1, 1997, p. 395.
[4] Goutiere V, Liu F, Charette A. JQSRT 2000;64:299.
[5] Ludwig DB, Malkmus W, Reardon JE, Thomson JAL. Handbook of infrared radiation from combustion gases. NASA SP3080, 1973.
[6] Soufiani A, Taine J. Int J Heat Mass Transfer 1997;40:987.
[7] Kim TK, Menart JA, Lee HS. J Heat Transfer 1991;113:946.
[8] Liu F, Smallwood GJ, Gülder ÖL. J Thermophys Heat Transfer 1999;13:285.
[9] Hottel HC, Sarofim AF. Radiative transfer. New York: McGraw-Hill, 1967, p. 247.
[10] Yang SS, Song TH. Int J Thermal Sci 1999;38:228.
[11] Lacis AA, Oinas V. J Geophys Res 1991;96:9027.
[12] Goody R, West R, Chen L, Crisp D. JQSRT 1989;42:539.
[13] Tang KC, Brewster MQ. In: Armaly BF, editor. ASME Proceedings of the Seventh AIAA/ASME Joint Thermophysics and Heat Transfer Conference, vol. 1, 1998, p. 32.
[14] Goody RM, Yung YL. Atmospheric radiation, 2nd ed. Oxford, UK: Oxford University Press, 1989.
[15] Rivière Ph, Soufiani A, Taine J. JQSRT 1992;48:187.
[16] Liu F. J Heat Transfer 1999;121:200.
[17] Liu F, Becker HA, Pollard A. Numer Heat Transfer Part B 1996:30:23.