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**Comonotonic global spectral models of gas radiation
in non-uniform media based on arbitrary probability
measures**

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Abstract.

The aim of the present work is to provide a universal theoretical formulation of global methods for radiative heat transfer in non-uniform gaseous media. Starting from the definition of an arbitrary probability measure on the wavenumber axis, it is shown that no gas reference state is required to develop rigorously a full spectrum model, both in uniform and non-uniform media.

This general formulation, which constitutes a novel mathematical modeling of gas radiation, is then applied for: 1/ the theoretical justification of new developments introduced recently in the so-called Rank Correlated SLW method in non-uniform media, 2/ emphasizing the differences and similarities between the SLW and FSK methods, from the point of view of the way these two techniques treat path non-uniformities.

The theoretical results provided in the present work can also be used to enlighten the concept of “spectral correlation”, widely encountered in gas radiation modeling.

Keywords. Gas radiation, global models, comonotonicity, copula, Rank Correlated SLW.

NOMENCLATURE

f function of the absorption coefficient

F k -distribution as defined by Eq. (3) or (4)

Gr rank transmutation mapping function, Eq. (5)

h “correlating” function, Eq. (25)

H Heaviside step function

I radiative intensity, Eq. (15)

$I_{b\eta}(T)$ spectral blackbody radiative intensity at temperature T and wavenumber η

$I_b(T) = \frac{\sigma T^4}{\pi}$ total blackbody radiative intensity, in $\text{W} \cdot \text{m}^{-2} \cdot \text{sr}^{-1}$

k absorption coefficient, in cm^{-1}

L gas path length, in cm

\mathcal{P} probability

s abscissa along a radiation path, in cm

T temperature, in K

Greek symbols

δ Dirac Delta function

Δk small increment of values of k , in cm^{-1}

η wavenumber, in cm^{-1}

κ_η spectral absorption coefficient, in cm^{-1}

ϕ gas thermodynamic state vector $\phi = \{ \text{temperature, species concentrations, total pressure} \}$

μ positive function used to define a measure on the wavenumber axis

ρ_s Spearman's rank correlation coefficient, Eqs. (26)

w weights of the quadratures in Eq. (10)

ξ random variable uniformly distributed over the interval $[0,1]$

Subscripts, superscripts

loc local state along a non-uniform path

P Planck mean

μ relative to the measure μ

ref reference

i,n quadrature index and order respectively

m,1,2 index representing a particular thermophysical state of the gas

Notation $\frac{dGr(X=x)}{dX}$ represents the value of the derivative of function *Gr* with respect to *X*

evaluated at $X = x$. It is equivalent to $\frac{dGr(X=x)}{dX} = \left[\frac{dGr(X)}{dX} \right]_{X=x}$.

1. INTRODUCTION

All existing global methods for the radiative properties of gases, such as ADF [1], SLW [2] or FSK [3], require the specification of some reference thermophysical state of the gas ϕ_{ref} , usually called a state vector and that encompasses all the quantities required to define a given state of the gas, *e.g.*, its temperature, species concentrations and total pressure. The reference state is used to « correlate » spectra at different locations along a non-uniform, *i.e.*, non-homogeneous non-isothermal, radiation path. The reference state ϕ_{ref} needs to be specified in all existing global methods to define reference full spectrum distribution functions (ALBDF in SLW terminology), on which all these techniques [1-3] are founded.

Many approaches [1-3] were proposed during the past decades to choose values for the reference state. However, none of them is fully founded on a systematic rigorous theoretical derivation. Consequently, it is widely recognized that no universal recommendation, other than that based on results obtained on some restricted set of test cases, can be made for general radiative heat transfer calculations in non-uniform gaseous media. We will show here that in fact no reference thermophysical state is actually required to develop a full spectrum gas radiation model. Recourse to sophisticated and mostly theoretically unjustified, but however pragmatic, techniques to define these parameters can thus be avoided.

Indeed, the main objective of the present work is to present a rigorous derivation of a general global method of gas radiation based on an arbitrary probability measure on the wavenumber axis. It does not require specification of the reference thermophysical state. The mathematical evidence is founded on the same tools as introduced in the ℓ -distribution approach [4], *i.e.*, rank transmutation maps and copulas that are two concepts taken from probability theory.

This paper is mostly theoretical. A number of applications of the theoretical development presented here has been presented in Ref. [5], where the Rank Correlated SLW model is

introduced. Consequently, only limited illustration through examples is included here. The present derivation can serve as a theoretical justification of the « correlated » methods in non-uniform media based on the assumption of rank correlated or comonotonic spectra which do not require specification of the reference state. Connections of the present derivations with the Rank Correlated SLW model [5] are emphasized at the end of the document. Ref. [5] provides extensive applications of the theoretical results developed in the present work and illustrates its relevancy for the building of new and efficient methods of gas radiation.

Finally, this work also has as its objective the careful introduction of the concept of spectral correlation. This problem, together with its engineering treatment, is undoubtedly one of the trickiest concepts in gas radiation modeling. Section 3 is specifically dedicated to this topic.

2. ABSORPTION LINE DISTRIBUTION FUNCTION

In this section, we consider radiative transfer in a uniform gaseous medium at state ϕ characterized by the spectral absorption coefficient $\kappa_\eta = \kappa_\eta(\phi)$.

In k -distribution methods, gas absorption spectra are treated as random variables with given distribution functions. It can be noticed that this statistical view was almost inexistent in the early works on k -distribution methods, including Ambartzumian's work [6]. It only became common when the notion of "correlation" between spectra was proposed to treat local variations in spectrum arising from gas non-uniformities [7]. "Correlation" is a concept which is fundamentally based on a probabilistic view of the problem.

The general definition of random variables provided, for instance, in Ref. [8] can be reformulated in terms of gas spectra as follows: as absorption coefficients are functions of wavenumbers, k -distributions are associated with a measure on the wavenumbers axis, *e.g.*, widths of spectral intervals. The definition of a measure can be interpreted in Monte Carlo terminology as the choice of a method to randomly sample wavenumbers.

Let us introduce the probability measure over the wavenumber axis as a non-negative

mathematically integrable function μ such that $\int_0^{+\infty} \mu(\eta) d\eta = 1$.

Let ξ , uniformly distributed over the $[0,1]$ interval and which will be referred to as a “germ”,

correspond to the output of some random number generator in a Monte Carlo approach.

Wavenumbers can be sampled with respect to the probability measure μ by application of the inverse transformation theorem, widely used in Monte Carlo methods [9] as:

$$\mathbb{P}[\eta' < \eta(\xi)] = \xi \quad (1)$$

where the probability with respect to μ for any wavenumber η' to be lower than a prescribed value η is defined as:

$$\mathbb{P}(\eta' < \eta) = \int_0^{\eta} \mu(\eta'') d\eta'' \quad (2)$$

This is illustrated in Figure 1.

FIGURE 1 HERE

It is possible to evaluate the probability with respect to measure μ for the spectral absorption coefficient $\kappa_{\eta} = \kappa_{\eta}(\phi)$ to be lower than a given prescribed value k by: 1/ sampling uniformly over the interval $[0,1]$ a large number N of values of ξ ; 2/ calculating the corresponding wavenumbers $\eta(\xi)$ by solving Eq. (2); 3/ evaluating the absorption coefficients $\kappa_{\eta(\xi)}$ at these randomly chosen spectral locations ; 4/ determining the amount $N(k)$ of such values that are lower than the prescribed limit k .

The probability $\mathbb{P}(\kappa_{\eta} < k)$ can then be estimated as the ratio $N(k)/N$.

When N approaches infinity, one then converges toward the following limit:

$$F_{\mu}(k) = \mathbb{P}(\kappa_{\eta} < k) = \int_0^{+\infty} H(\kappa_{\eta} - k) \mu(\eta) d\eta \quad (3)$$

where H is the Heaviside step function which is 0 if $\kappa_{\eta} - k < 0$ and 1 if $\kappa_{\eta} - k > 0$. It indicates the membership of a given wavenumber to the set $\{\eta : \kappa_{\eta} < k\}$. The use of the Heaviside function in Eq. (3) mostly formalizes the continuous limit, for large values of N , of the counting process used in step 4/.

By Eq. (3), the Absorption Line Distribution Function (ALDF) with respect to μ , that corresponds to the k -distribution, is defined. When the measure $\mu(\eta) = I_{b\eta}(T)/I_b(T)$, the ALDF is called the Absorption Line Blackbody Distribution function (ALBDF) [2].

3. RANK TRANSMUTATION MAPS AND WEIGHTS

Now, let us assume that we want to evaluate the following integral, where $f(k)$ is any regular

function of the absorption coefficient: $\int_0^{+\infty} f(\kappa_{\eta}) I_{b\eta}(T) d\eta$. Then, according to full spectrum k -

distribution methods:

$$\int_0^{+\infty} f(\kappa_{\eta}) I_{b\eta}(T) d\eta = \frac{\sigma T^4}{\pi} \int_0^{+\infty} f(k) dF(k) \quad (4)$$

where $F(k) = \frac{\pi}{\sigma T^4} \int_0^{+\infty} H(k - \kappa_{\eta}) I_{b\eta}(T) d\eta = \frac{1}{I_b(T)} \int_0^{+\infty} H(k - \kappa_{\eta}) I_{b\eta}(T) d\eta$.

Here, $F = F(k)$ represents the fraction of blackbody intensity at temperature T emitted in the spectral regions over which the spectral absorption coefficient $\kappa_{\eta} = \kappa_{\eta}(\phi)$ takes values lower

than k . $F(k)$ is a particular case of function $F_\mu(k)$ for which the measure $\mu(\eta) = I_{b\eta}(T)/I_b(T)$.

Let us construct a function, mathematically called a rank transmutation map [10], defined as:

$$Gr(X) = F[F_\mu^{-1}(X)], X \in [0,1] \quad (5)$$

The function Gr maps the interval $[0,1]$ onto itself, and is such that:

$$F(k) = Gr[F_\mu(k)] \quad (6)$$

The principle of the definition of the rank transmutation map Gr is illustrated Figures 2 - 4.

FIGURE 2 HERE

FIGURE 3 HERE

FIGURE 4 HERE

Both sides of Eq. (6) can be differentiated with respect to k to give:

$$\frac{dF(k)}{dk} = \frac{dF_\mu(k)}{dk} \frac{dGr[X = F_\mu(k)]}{dX} \quad (7)$$

From Eq. (7), it is noted that the function Gr is strictly increasing because F_μ and F are two distribution functions both increasing with respect to the variable k , and thus that Gr can be inverted.

Eq. (7) can be used inside Eq. (4) to yield:

$$\begin{aligned} \int_0^{+\infty} f(\kappa_\eta) I_{b\eta}(T) d\eta &= I_b(T) \int_0^{+\infty} f(k) dF(k) \\ &= I_b(T) \int_0^{+\infty} f(k) \frac{dGr[X = F_\mu(k)]}{dX} dF_\mu(k) \\ &= I_b(T) \int_0^1 f[k(\xi)] \frac{dGr(X = \xi)}{dX} d\xi \end{aligned} \quad (8)$$

The last equality in Eq. (8) arises from the inversion of Eq. (5) $F_\mu[k(\xi)] = \xi = Gr^{-1}(F[k(\xi)])$

which is related to the inverse transformation theorem.

Now let us choose $f(k)$ so that Eq. (4) represents the total transmissivity of a gas path of length L , e.g., $f(k) = \exp(-kL)$ (notice that the same method applies to any function of the variable k). We obtain in this situation:

$$\int_0^{+\infty} \exp(-\kappa_\eta L) I_{b\eta}(T) d\eta = I_b(T) \int_0^1 \exp[-k(\xi)L] \frac{dGr(X=\xi)}{dX} d\xi \quad (9)$$

This integral can be approximated using any numerical quadrature of order n on the $[0,1]$ interval. If the weights and abscissas of the quadrature are w_i and x_i respectively, we have:

$$\int_0^{+\infty} \exp(-\kappa_\eta L) I_{b\eta}(T) d\eta \approx I_b(T) \sum_{i=1}^n w_i \frac{dGr(X=x_i)}{dX} \exp[-k(x_i)L] \quad (10)$$

Eq. (10) has the same mathematical form as full spectrum weighted sum of gray gases models shown as

$$\int_0^{+\infty} \exp(-\kappa_\eta L) I_{b\eta}(T) d\eta \approx I_b(T) \sum_{i=1}^n a_i \exp[-k(x_i)L] \quad (11)$$

but in which the weights are

$$a_i = w_i \frac{dGr(X=x_i)}{dX} \quad (12)$$

and where the values of the absorption coefficients $k(x_i)$ are defined, from Eq. (5), as the solution of:

$$Gr(x_i) = F[F_\mu^{-1}(x_i)] = F[k(x_i)] \quad (13)$$

It can be noticed that:

- if the function $\mu(\eta) = I_{b\eta}(T)/I_b(T)$, which is a measure which defines F_μ , is chosen then the previous relationships provide $Gr(X) = X$ and $k(X) = F^{-1}(X)$ which gives the same result as full spectrum k -distribution models in uniform media;

- more generally, if $\mu(\eta) \neq I_{b\eta}(T)/I_b(T)$, as is for instance used in the so-called LBL PMC approach [3] for which the measure on the wavenumber axis is defined as

$$\mu(\eta) = \frac{\kappa_\eta I_{b\eta}(T)}{\int_0^{+\infty} \kappa_\eta I_{b\eta}(T) d\eta},$$

then the method allows formulating the model in a way which

is similar to common approaches. The only distinction then is that the choice of the measure on the wavenumber axis is not the same as these usual global models.

- if some reference source temperature T_0 is defined, and one chooses $\mu(\eta) = I_{b\eta}(T_0)/I_b(T_0)$, we obtain the usual FSK and Generalized SLW model weights in uniform and non-uniform media [11] as we then have, with the notation

$$F_0(k) = \frac{1}{I_b(T_0)} \int_0^{+\infty} H(k - \kappa_\eta) I_{b\eta}(T_0) d\eta:$$

$$\frac{dGr(X)}{dX} = \frac{\frac{dF[Y = F_0^{-1}(X)]}{dY}}{\frac{dF_0[Y = F_0^{-1}(X)]}{dY}} \Rightarrow \frac{dGr(X = \xi)}{dX} \underset{F_0^{-1}(\xi)=k(\xi)}{=} = \frac{dF[k(\xi)]}{dk(\xi)} \quad (14-a)$$

$$\frac{dGr(X)}{dX} = \frac{\frac{dF[Y = F_0^{-1}(X)]}{dY}}{\frac{dF_0[Y = F_0^{-1}(X)]}{dY}} \Rightarrow \frac{dGr(X = \xi)}{dX} \underset{F_0^{-1}(\xi)=k(\xi)}{=} = \frac{\frac{dF[Y = k(\xi)]}{dY}}{\frac{dF_0[Y = k(\xi)]}{dY}} \quad (14-b)$$

Eqs. (14) shows that the weights in generalized SLW (14-a) and FSK (14-b) methods are rigorously equivalent, as the only difference between the two approaches lies in the mathematical form chosen to write dGr/dX . Notice that we have used to write Eq. (14-a):

$$F_0[k(\xi)] = \xi \Rightarrow \frac{dF_0[k(\xi)]}{dk(\xi)} dk(\xi) = d\xi \Rightarrow \frac{1}{\frac{dF_0[k(\xi)]}{dk(\xi)}} = \frac{dk(\xi)}{d\xi} \quad (14-c)$$

Developments provided in this section show that the measure on the wavenumber axis does not explicitly require the definition of some reference Planck temperature, as shown in Eq. (2). This reference source temperature is only used in the definition of the probability measure over the wavenumber axis, and thus represents only one possible way to sample wavenumbers and define probability laws. This finding is significant, since it relieves global methods theoretically from the requirement that a reference state be specified.

From Eq. (9) it can be readily shown that the differential form of the Radiative Transfer Equation, RTE, associated with the present theoretical development is

$$\frac{dI(\xi, s)}{ds} = -k(\xi)I(\xi, s) + k(\xi) \frac{dGr(X = \xi)}{dX} I_b(T) \quad (15-a)$$

and the total radiative intensity is

$$I(s) = \int_0^{+\infty} I_\eta(s) d\eta = \int_0^1 I(\xi, s) d\xi \quad (15-b)$$

It is interesting to note that with the specific choice $\mu(\eta) = \frac{\kappa_\eta I_{b\eta}(T)}{\int_0^{+\infty} \kappa_\eta I_{b\eta}(T) d\eta} = \frac{\kappa_\eta}{k_p} \frac{I_{b\eta}(T)}{I_b(T)}$,

which corresponds to the probability measure used in the so-called LBL Photon Monte Carlo method – LBL PMC [12], one obtains the RTE formulation:

$$\frac{dI(\xi, s)}{ds} = -k(\xi)I(\xi, s) + k_p I_b(T) \quad (15-c)$$

where k_p is the Planck mean absorption coefficient. It should be noted that, in this case, values of $k(\xi)$ need to be sampled from $F_{\kappa_\eta I_{b\eta}(T)/k_p I_b(T)}$ which is not the usual ALDBF.

4. EXTENSION TO NON-UNIFORM GASES

Up to now our analysis has mostly concerned uniform gaseous media. In this section, as more than one thermophysical state of the gas will be considered in real applications, we will use the following notations: κ_η^m will represent the spectral absorption coefficient in the thermophysical state ϕ_m . The corresponding distribution will be written $F_\mu^m(k) = F_\mu(k, \phi_m)$. The joint distribution for two thermophysical states ϕ_1 and ϕ_2 will be denoted $F_\mu^{12}(k_1, k_2) = F_\mu(k_1, \phi_1; k_2, \phi_2)$.

4.1. Statistical dependence model

Let us consider a pair of thermophysical states represented by two absorption coefficients, κ_η^1 and κ_η^2 and choose arbitrarily two positive real numbers k_1 and k_2 . As in the previous section, we can define the joint probability of the “event” $\{\kappa_\eta^1 < k_1 \text{ and } \kappa_\eta^2 < k_2\}$ from Eq. (3) as,

$$\begin{aligned} F_\mu^{12}(k_1, k_2) &= \mathbb{P}(\kappa_\eta^1 < k_1 \text{ and } \kappa_\eta^2 < k_2) = \int_0^{+\infty} H(\kappa_\eta^1 - k_1) H(\kappa_\eta^2 - k_2) d\mathbb{P}[\eta < \eta(\xi)] \\ &= \int_0^{+\infty} H(\kappa_\eta^1 - k_1) H(\kappa_\eta^2 - k_2) \mu(\eta) d\eta \end{aligned} \quad (16)$$

Then, from the definition of the Heaviside step function, the two following inequalities hold:

$$\begin{aligned} \mathbb{P}(\kappa_\eta^1 < k_1 \text{ and } \kappa_\eta^2 < k_2) &= \int_0^{+\infty} H(\kappa_\eta^1 - k_1) \underbrace{H(\kappa_\eta^2 - k_2)}_{\leq 1} d\mathbb{P}[\eta < \eta(\xi)] \\ &\leq \int_0^{+\infty} H(\kappa_\eta^1 - k_1) \mu(\eta) d\eta = \mathbb{P}(\kappa_\eta^1 < k_1) = F_\mu^1(k_1) \end{aligned} \quad (17)$$

and:

$$\begin{aligned}
\mathbb{P}(\kappa_\eta^1 < k_1 \text{ and } \kappa_\eta^2 < k_2) &= \int_0^{+\infty} \underbrace{H(\kappa_\eta^1 - k_1)}_{\leq 1} H(\kappa_\eta^2 - k_2) d\mathbb{P}[\eta < \eta(\xi)] \\
&\leq \int_0^{+\infty} H(\kappa_\eta^2 - k_2) \mu(\eta) d\eta = \mathbb{P}(\kappa_\eta^2 < k_2) = F_\mu^2(k_2)
\end{aligned} \tag{18}$$

Eqs. (17-18) can be combined into a single equation:

$$\mathbb{P}(\kappa_\eta^1 < k_1 \text{ and } \kappa_\eta^2 < k_2) \leq \min\{\mathbb{P}(\kappa_\eta^1 < k_1); \mathbb{P}(\kappa_\eta^2 < k_2)\} \tag{19}$$

As soon as one of the two following relations holds $\{\eta: \kappa_\eta^1 < k_1\} \subseteq \{\eta: \kappa_\eta^2 < k_2\}$ or

$\{\eta: \kappa_\eta^2 < k_2\} \subseteq \{\eta: \kappa_\eta^1 < k_1\}$, then the following relationship is verified:

$$F_\mu^{12}(k_1, k_2) = \min\{F_\mu^1(k_1), F_\mu^2(k_2)\} = \begin{cases} F_\mu^1(k_1) & \text{if } F_\mu^1(k_1) < F_\mu^2(k_2) \\ F_\mu^2(k_2) & \text{if } F_\mu^2(k_2) < F_\mu^1(k_1) \end{cases} \tag{20}$$

We will focus now our attention on the special case set by Eq. (20), which corresponds to the equality in Eq. (19).

By differentiating Eq. (20) with respect to k_1 for instance, as symmetrical relationships can be obtained if we differentiate first with respect to k_2 , we find:

$$\frac{\partial F_\mu^{12}(k_1, k_2)}{\partial k_1} = \begin{cases} \frac{\partial F_\mu^1(k_1)}{\partial k_1} & \text{if } F_\mu^1(k_1) < F_\mu^2(k_2) \\ 0 & \text{if } F_\mu^2(k_2) < F_\mu^1(k_1) \end{cases} \tag{21}$$

Using again the definition of the Heaviside step function, these two relationships can be summarized into:

$$\frac{\partial F_\mu^{12}(k_1, k_2)}{\partial k_1} = H[F_\mu^2(k_2) - F_\mu^1(k_1)] \frac{\partial F_\mu^1(k_1)}{\partial k_1} \tag{22}$$

Then, differentiation of Eq. (22) with respect to k_2 yields:

$$\frac{\partial^2 F_\mu^{12}(k_1, k_2)}{\partial k_1 \partial k_2} = \delta[F_\mu^2(k_2) - F_\mu^1(k_1)] \frac{\partial F_\mu^1(k_1)}{\partial k_1} \frac{\partial F_\mu^2(k_2)}{\partial k_2} \quad (23)$$

where δ is the Dirac delta function.

This shows that Eq. (23) is valid as soon as one of the two following relationships holds:

$$\{\eta : \kappa_\eta^1 < k_1\} \subseteq \{\eta : \kappa_\eta^2 < k_2\} \text{ or } \{\eta : \kappa_\eta^2 < k_2\} \subseteq \{\eta : \kappa_\eta^1 < k_1\}.$$

Eq. (23) can be analyzed as follows: the finite increment form of the left-hand side represents the probability, divided by the product $\Delta k_1 \Delta k_2$, for the spectral absorption coefficients κ_η^1 and κ_η^2 to be simultaneously inside small intervals of widths Δk_1 and Δk_2 around k_1 and k_2 . The

Dirac function at the RHS means that this probability is null almost everywhere except when:

$$F_\mu^2(k_2) = F_\mu^1(k_1) \quad (24)$$

This last equation thus defines the statistical dependence that exists between the two spectra as soon as Eq. (20) holds. Indeed, it means that once a value for k_1 that represents the absorption coefficient in the first state is chosen, then the value of the absorption coefficient in state 2 cannot be considered as arbitrary but must comply with the implicit equation (24).

Eq. (24) can be further analyzed using *C*-curves which are parametric plots, with respect to parameter η , in the $X = \kappa_\eta^1$, $Y = \kappa_\eta^2$ plane depicting the relationships between spectra [13]. If

Eq. (24) holds, then the set of points defined implicitly as $F_\mu^2(\kappa_\eta^2) - F_\mu^1(\kappa_\eta^1) = 0$ which characterizes the *C*-curve corresponds to an increasing function h whose equation is given explicitly as:

$$\kappa_\eta^2 = h(\kappa_\eta^1), \text{ where } h(k) = (F_\mu^2)^{-1}[F_\mu^1(k)] \quad (25)$$

It can be observed that:

- Equality (24) is similar to the implicit equation encountered in full spectrum models, involving the ALBDF in the SLW approach, but formulated here in terms of an arbitrary measure over the wavenumber axis.
- If, for instance, the first state (superscript “1”) is called a “reference”, then one obtains by Eq. (24) or equivalently Eq. (25) the so-called “reference approaches”, see Table 1. The “correlating” function required in the FSK method is then given explicitly by Eq. (25) with the specific choice $\mu(\eta) = I_{b\eta}(T_{ref})/I_b(T_{ref})$ where T_{ref} is a prescribed reference source temperature.
- The “correlating” function h is defined in terms of the $\mu(\eta)$ function, see Eq. (25). This means that when $\mu(\eta) = I_{b\eta}(T_{ref})/I_b(T_{ref})$, the h function involves ALBDFs evaluated at the same reference source temperature.

TABLE 1 HERE

4.2. Relationship with copula’s theory

Most of the results presented in this section can be obtained directly if one invokes copula’s theory [14].

A two-dimensional copula is a bi-variate probability distribution function $C(X,Y):[0,1]\times[0,1]\rightarrow[0,1]$ increasing in each of its variables and such that $C(0,Y)=C(X,0)=0$ and $C(X,1)=X$, $C(1,Y)=Y$. It was shown by Sklar [15] that any bi-variate distribution function, such as Eq. (16), can be written by combining a copula with the distribution functions associated with the single variables, taken separately as

$$F_{\mu}^{12}(k_1, k_2) = C[F_{\mu}^1(k_1), F_{\mu}^2(k_2)].$$

Eq. (20) corresponds to the definition of the upper Frechet-Hoeffding bound copula $C(X,Y) = \min\{X,Y\}$ and defines random variables, otherwise known as spectra in k -distribution methods, which are called comonotonic (for common monotonicity).

The Spearman rank correlation coefficient measures the non-linear dependency between random variables. It can be obtained directly from the copula [16] as:

$$\begin{aligned}\rho_s &= 12 \int_0^1 \int_0^1 C(X,Y) dX dY - 3 \\ &= 12 \int_0^1 \int_0^1 XY \frac{\partial^2 C(X,Y)}{\partial X \partial Y} dX dY - 3\end{aligned}\tag{26-a}$$

The coefficient ρ_s is equal to 1 in the case of comonotonic variables, *i.e.*, when

$$\frac{\partial^2 C(X,Y)}{\partial X \partial Y} = \delta(X - Y):$$

$$\begin{aligned}\rho_s &= 12 \int_0^1 \int_0^1 XY \delta(X - Y) dX dY - 3 \\ &= 12 \int_0^1 X^2 dX - 3 \\ &= 1\end{aligned}\tag{26-b}$$

Comonotonicity thus complies with the original definition of “correlation” between spectra as “rank correlation”, as described in Ref. [7] which is, to the best of our knowledge, the first to introduce the concept of “correlated” spectra.

The main interest in thinking of the problem in terms of comonotonicity is that mathematically, two random variables are comonotonic *if and only if* they can be written as strictly increasing functions of a single “germ” random variable [17]. This simply means that any absorption coefficients at a local states, index *loc*, along a non uniform path can be obtained from the same uniform random variable ξ over the [0,1] interval as:

$$k_{loc}(\xi) = [F_{\mu}^{loc}]^{-1}(\xi) \quad (27)$$

This allows the representation of the statistical dependence between spectra through the use of this unique variable ξ . As a consequence this avoids recourse to any reference state.

The so-called ‘‘Rank Correlated Generalized SLW model’’ is essentially founded on this last theorem [17]. These developments justify theoretically the approach provided in section 2.1 from Ref. [5] which does not require the definition of any reference state.

The present method also generalizes to the full spectrum the technique used over narrow bands, over which no reference state needs to be defined but the treatment of non-uniformities is however based on the same model of statistical dependence between spectra in distinct states as used here. However, over narrow bands, the formulation is simpler because the most natural way to sample wavenumbers is uniformly: no weighting by a Planck function or use of some specific $\mu(\eta)$ function has a sense, as it would unnecessarily complicate the problem.

5. THE RANK CORRELATED GENERALIZED SLW MODEL

It is beyond the scope of the present work to try to define what should be the best choice for function $\mu(\eta)$. There are multiple possibilities. However, some of the developments provided here were used recently to propose a new formulation of the SLW model that does not require the specification of a reference state of the gas. This model, together with its connections with the SLW and FSK reference approaches, is described in this section. Details about this new SLW technique can be found in Ref. [5].

As noticed in Section 2, the Generalized SLW and FSK approaches are rigorously the same in uniform media, as they correspond to two different ways to write the mapping function Gr , Eqs. (14). In these two models the definition of the function $\mu(\eta) = \mu(\eta, T_{ref})$ requires the choice of a reference blackbody source temperature T_{ref} . We will restrict our discussion to this

particular case in this section and use $\mu(\eta) = \mu(\eta, T_{ref}) = I_{b\eta}(T_{ref}) / I_b(T_{ref})$, which corresponds to the usual way this function is defined in these methods.

The subtle difference between these two models lies in the way “correlation” between spectra is introduced. Indeed, in the FSK method “correlation” assumes the existence of an increasing function, written k_{η}^* in ref. [3] (see Eq. (20.116)), that associates gas spectra in distinct states. In the Generalized SLW intervals of wavenumbers are assumed to be kept unchanged for given fixed values of the absorption coefficient in the different states. Maintaining the same spectral intervals allows avoiding the appearance of Leibniz terms when spectral integrals are evaluated over non-uniform paths. Both methods are equivalent as they lead to the same dependence structure, mathematically formalized by Eqs. (20-25). However, from a pure technical perspective, FSK is formulated in a way which is similar to Eq. (25), requiring the explicit definition of a reference state, whereas SLW is closer to Eq. (24) in the sense that it only uses relationships between spectral intervals associated with distinct states.

Both approaches are rigorously the same, as soon as some reference gas spectrum is chosen. Indeed, in this situation, the reference spectrum is used to provide some discretization of the interval of k -values in the reference state, and the spectral intervals used for the “correlation” are then set by these fixed k -values. Notice that the FSK method as it has been formulated to date cannot omit the definition of a reference state, due to the way the treatment of non-uniformities is handled with regard to some functional relationship between gas spectra.

What is different in the Rank Correlated SLW model is the way spectral intervals are defined to construct gray gases. Indeed, in this model they are obtained by solving Eq. (27), that is directly related to the inverse transformation theorem, by using the same “germ” random variable ξ to generate gray gas spectra in all thermophysical states.

This simply means that according to the assumption of rank correlation, *i.e.*, comonotonicity of gas spectra, only a discretization of the interval of variations of the “germ” ξ is required to define: 1/ the gray gases absorption coefficients in any state and, as a consequence, 2/ the spectral intervals over which gas spectra are assumed to be constant. Consequently, they are considered to be the same for any state and do not depend on the choice of any reference thermophysical condition. This is illustrated in Figure 5 (General case) and Figure 6 (Rank Correlated SLW approach).

One can notice that the way the Rank Correlated SLW model was introduced in Ref. [5] may look somewhat different than the method proposed here. A comment is given here to clarify this point.

The definition of the spectral intervals in the RC-SLW model is based on the following assumption of relationship, similar to Eqs. (A3.1) from Ref. [5], and already introduced in Section 4.1:

$$\{\eta : \kappa_{\eta}^1 < k_1\} \subseteq \{\eta : \kappa_{\eta}^2 < k_2\} \text{ or } \{\eta : \kappa_{\eta}^1 < k_1\} \supseteq \{\eta : \kappa_{\eta}^2 < k_2\} \quad (28)$$

where k_1 and k_2 are two arbitrary possible values of the absorption coefficient.

Let us assume that k_1 and k_2 are such that the first inclusion applies. In this case, using Eq. (16) from the present work, one obtains:

$$\begin{aligned} \mathbb{P}(\kappa_{\eta}^1 < k_1 \text{ and } \kappa_{\eta}^2 < k_2) &= \int_{\{\eta : \kappa_{\eta}^1 < k_1\} \cap \{\eta : \kappa_{\eta}^2 < k_2\}} \mu(\eta, T_{ref}) d\eta \\ &= \int_{\{\eta : \kappa_{\eta}^1 < k_1\}} \mu(\eta, T_{ref}) d\eta \\ &= F_{\mu(\eta, T_{ref})}^1(k_1) \end{aligned} \quad (29-a)$$

Symmetrically, if the second inclusion is true the following relation holds:

$$\begin{aligned}
\mathbb{P}(\kappa_{\eta}^1 < k_1 \text{ and } \kappa_{\eta}^2 < k_2) &= \int_{\{\eta: \kappa_{\eta}^1 < k_1\} \cap \{\eta: \kappa_{\eta}^2 < k_2\}} \mu(\eta, T_{ref}) d\eta \\
&= \int_{\{\eta: \kappa_{\eta}^2 < k_2\}} \mu(\eta, T_{ref}) d\eta \\
&= F_{\mu(\eta, T_{ref})}^2(k_2)
\end{aligned} \tag{29-b}$$

This means that if Eq. (28) holds, then one of the two equations (29) is true. This shows that Eq. (28) can be rewritten equivalently as:

$$\mathbb{P}(\kappa_{\eta}^1 < k_1 \text{ and } \kappa_{\eta}^2 < k_2) = \min\{\mathbb{P}(\kappa_{\eta}^1 < k_1); \mathbb{P}(\kappa_{\eta}^2 < k_2)\} \tag{30}$$

which is Eq. (20).

FIGURE 5 HERE

FIGURE 6 HERE

Application of this new SLW model to radiative heat transfer calculations over a wide range of benchmarks can be found in Ref. [5]. We propose here an additional example that illustrates the strength of the method as an illustration of one of many possible theoretical approaches using the theoretical development presented here.

The case considered was initially proposed in Ref. [18] as one which is challenging for modelling with the ADF (Absorption Distribution Function) method. It consists of a mixture of H₂O and N₂ at constant water molar fraction 0.1. The gas temperature is described by the triangular profile depicted in Figure 7. It is maximum at the center of the medium (2500 K) and minimum at the two boundaries (500 K). The gas is surrounded by black walls at 500 K. The distance between the walls is $L = 2H = 0.4$ m. This example problem features very high spatial temperature gradients, designed to test the models developed previously and that based on the general theoretical development here. In Figure 8 results of comparisons between LBL calculations based on the HITEMP2010 spectroscopic database, and the original SLW model

using the reference approach proposed in Ref. [2] are provided. Two reference temperatures were considered for the comparison: 1/ the maximum temperature of the gas, $T_{max} = 2500$ K; and 2/ the volume-average temperature $T_{average} = 1000$ K. There are, of course, other possible definitions of the reference temperature. These two are selected simply to illustrate the sensitivity of the predictions. In this situation, the choice of the reference state has an important impact on the results with maximum relative errors that reach 10% for the reference temperature equal to T_{max} , and as high as 50% for the reference temperature $T_{average}$ selected. This leads to the conclusion that there may be some optimal choice for the reference state. In Figure 9, the same kind of comparison is made between LBL calculations and the RC-SLW model (based on the theoretical development here which does not require specification of a reference state). From this figure, one can observe that the change in the blackbody source temperature results in relative errors below 10% and 4%, respectively, for the reference temperatures T_{max} and $T_{average}$ selected.

The following conclusions can thus be drawn: 1/ the RC-SLW model provides more accurate results than the original SLW model based on a reference state ; 2/ results on radiative powers are almost insensitive to the choice of the blackbody source temperature. This second point suggests that the choice of the measure, when it depends on a reference blackbody source temperature, does not have a significant impact on the quality of the model's output in terms of radiative powers.

FIGURE 7 HERE

FIGURE 8 HERE

FIGURE 9 HERE

Local thermodynamic states of the problems considered differ only by the value of the gas temperature, and therefore, the reference state is defined by the choice of temperature T_{ref} .

The Rank Correlated SLW model based on the comonotonicity definition of spectra correlation does not use the reference temperature T_{ref} , but this formulation requires the specification of the blackbody source temperature T_b if the probability measure is defined with the help of the Planck blackbody spectral emissive power $\mu(\eta) = \mu(\eta, T_b) = I_{b\eta}(T_b)/I_b(T_b)$ as is usual for the SLW method.

It is interesting to investigate the sensitivity of the original Reference Approach SLW (RA-SLW) to the choice of the reference temperature T_{ref} and compare it to sensitivity to the choice of the blackbody source temperature T_b for the RC-SLW method, and assess their overall performance. This analysis can be performed for the example problem examined here with the help of the spatially averaged relative absolute error of prediction of the total divergence of the net radiative flux defined by the following equation:

$$Relative\ Error = \frac{1}{L \cdot \max |Q_{LBL}(x)|} \cdot \int_0^L |Q_{SLW}(x) - Q_{LBL}(x)| dx \cdot 100, \text{ in \%}$$

The dependence of the average error on T_{ref} for the RA-SLW method (where T_{ref} and T_b are taken to be identical) and on T_b for the RC-SLW method in the range from the minimum gas temperature in the layer to the temperature higher than the maximum temperature is presented in Figure 10.

FIGURE 10 HERE

For this example problem the relative error of the RA-SLW method depends strongly on T_{ref} , varying between 4% to 35%, with the lower values corresponding to higher values of the gas temperature in the medium (the minimum error value 4% is attained at about $T_{ref} = 2000K$).

Some sort of optimization routine may be needed to find the reference state which provides this best prediction.

By contrast, the minimum relative error of RA-SLW method is the maximum error of the RC-SLW method. The smallest values of relative error for RC-SLW correspond to the blackbody source temperature near the spatial average gas temperature of the layer (with the minimum value of 1.34 % at $T_b = 750 K$). However, in general, the RC-SLW is rather insensitive to the choice of T_b . As can be seen from Figure 10, any value of T_b will yield an error below 4% percent, and all of them are below the optimal result of the traditional RA-SLW method which can be obtained by optimization.

It can thus be concluded that the overall performance of the RC-SLW method is better than the performance of traditional SLW reference approach even without the necessity of optimization process. This confirms that for the problem considered, the Rank Correlated SLW spectral model based on the comonotonicity principle is the best spectral model, which yields the best possible prediction of the radiation transfer in non-isothermal gaseous medium.

6. CONCLUSION

The purposes of the present work were threefold: 1/ to develop a universal global model theory based on an arbitrary measure on the wavenumber axis, 2/ to use this general form to justify the method used in the so-called Rank Correlated Generalized SLW model [5], 3/ to introduce some tools that may be helpful to understand and formalize the concept of correlation between spectra in distinct thermophysical states.

It was shown that global models can be formulated rigorously without any need to specify either a blackbody source temperature or a gas reference state. This was done by : 1/ formulating the

global models in terms of an arbitrary probability measure on the wavenumber axis such that the dependence of global methods for the radiative properties of gases with the source blackbody temperature arises from the usual ways to define this measure, 2/ studying in detail the statistical dependency model between spectra in distinct states involved in all full spectrum approaches and usually referred to as « correlation ». We have shown here that this dependence model is called in copula's theory comonotonicity, and that this concept can be used in gas radiation modeling to show that no reference state is actually required to develop rigorously an approximate treatment of non-uniformities. The present derivation thus greatly simplifies the building of full spectrum models, as well as their practical implementation, as they do not depend anymore on any « a priori » definition of their building parameters. Furthermore, the approach complies with existing methods, which are in fact combinations of the RTE set by Eqs. (15-a,15-b), some method to evaluate the “local” weights, Eqs. (12,14), and to “correlate” spectra, Eq. (24) . The fundamental theoretical development presented here led us to propose a new and efficient SLW approach that does not require the specification of a gas reference state: the Rank Correlated Generalized SLW modeling [5]. The RC-SLW approach is a preferred possible spectral model which does not require a reference state, although the accuracy still remains slightly dependent on the choice of the reference blackbody source temperature which still suggests some optimization. The approach developed in the present paper, which can use any probability measure, provides all the theoretical foundations required to formulate and solve this issue.

Indirectly, the present paper also shows that any absorptivity, *i.e.*, ℓ -distribution [4,19], and k , *i.e.*, k -distribution, based model can be introduced using the same restricted set of statistical tools: rank transmutation maps and copulas. The connection with copulas theory: 1/ appears rather naturally within the frame of both k - and ℓ - distribution modellings; 2/ allows the direct use of many theorems and mathematical results already proved in the mathematical community

and that would be otherwise quite difficult or unintuitive to justify in non-uniform gas radiation modelling. Consequently, to some extent it thus simplifies the treatment of path-dependent non-uniformities more than it actually complicates the problem. The present work is an illustration of this fact: “correlation” used in gas radiation modelling for many years strictly coincides with the statistical concept of “comonotonicity” (both methods assume Spearman’s coefficients between gas spectra to be 1, viz. that any pair of gas spectra can be related through a strictly increasing function). Results related to comonotonic variables show that no reference state is actually required to build a full spectrum “correlated” model. This simplifies the building of such models without neither reducing the accuracy of the approach significantly nor involving an increase in its computational cost.

ACKNOWLEDGMENTS. This work was supported by the French National Research Agency under the grant ANR-12-BS09-0018 SMART-LECT.

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LIST OF TABLES

Method	Methodology / assumptions
FSK [3]	<ol style="list-style-type: none"> 1. Start with the definition of a reference state ϕ^{ref} . 2. Assume that any spectrum can be written as a strictly monotonous function of the reference absorption spectrum.
SLW reference approach [2]	<ol style="list-style-type: none"> 1. Start with the definition of a reference state. 2. Use the corresponding spectrum to discretize the wavenumber axis. 3. Assume that the same intervals can be used for any other states.
Rank correlated SLW [5]	<ol style="list-style-type: none"> 1. Assume the existence of a “germ” random variable / function. 2. Assume that any spectrum can be written as a strictly monotonous function of the “germ” – this is the assumption of rank correlation / co-monotonicity, as defined by Eq. (26) -. 3. Then any state can be used to discretize the wavenumber axis. 4. Use the same intervals for all thermophysical states.

TABLE 1. Similarities and differences between reference approaches and the rank correlated SLW model. See also Ref. [11].

LIST OF FIGURES

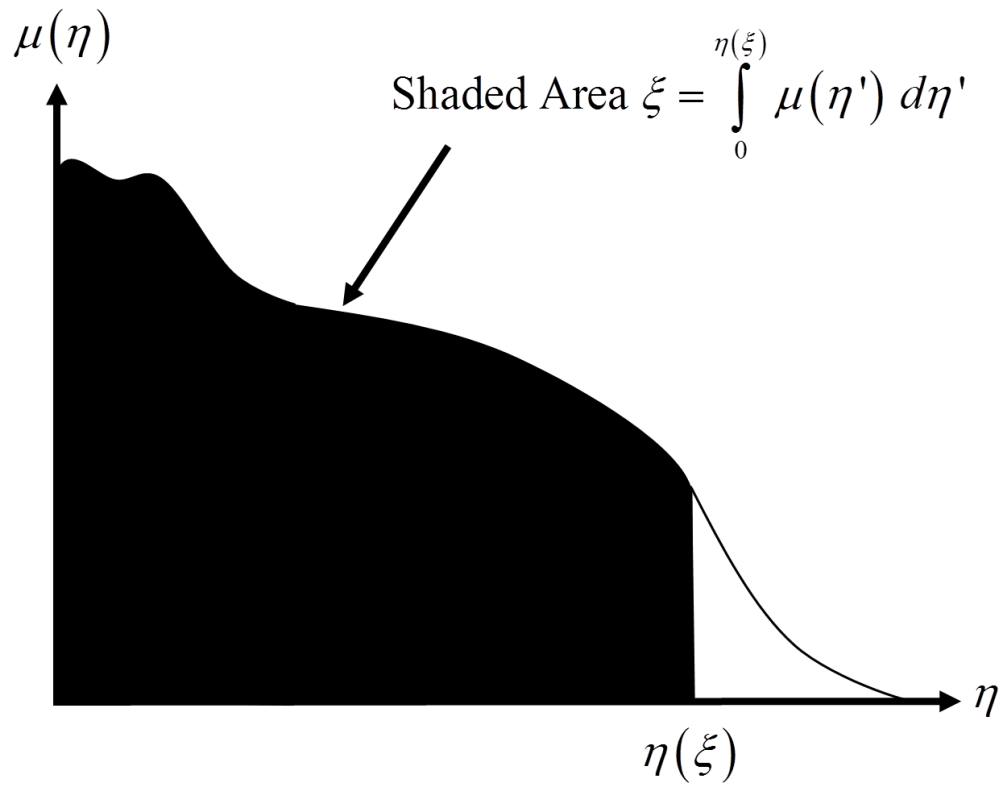


FIGURE 1. Illustration of the method to sample randomly spectral locations along the

wavenumber axis. $\int_0^{+\infty} \mu(\eta) d\eta = 1.$

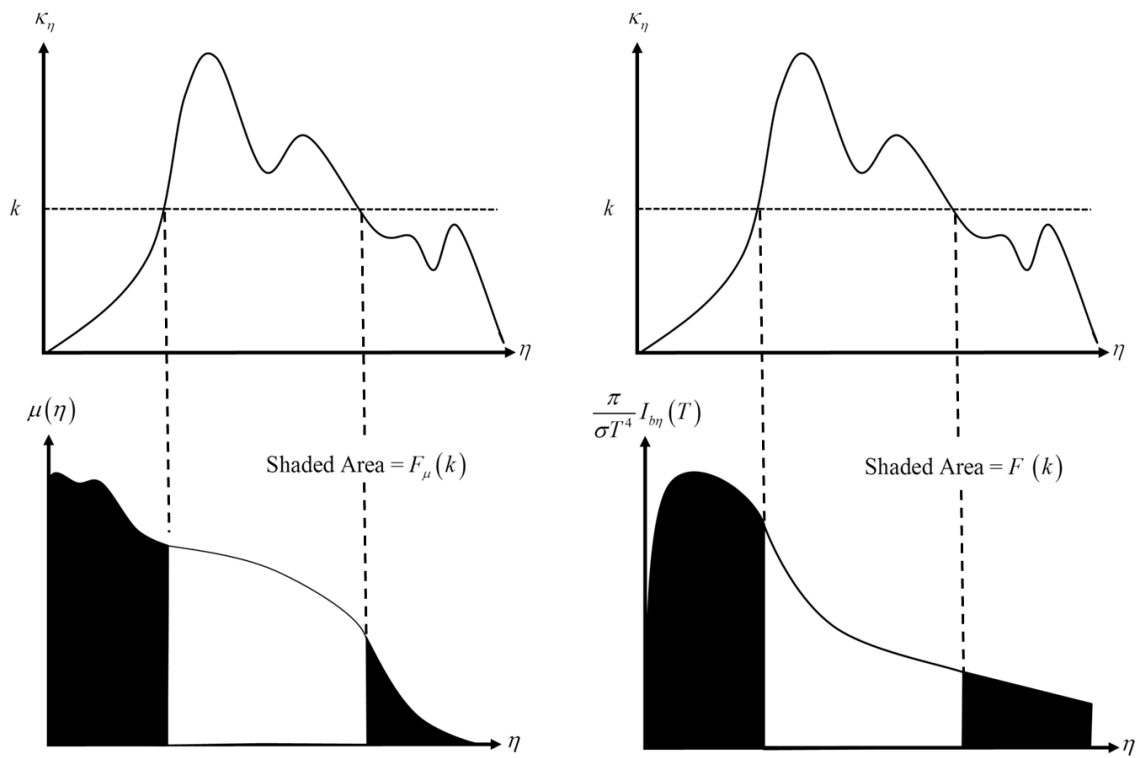


FIGURE 2. Definition of functions F_μ and F .

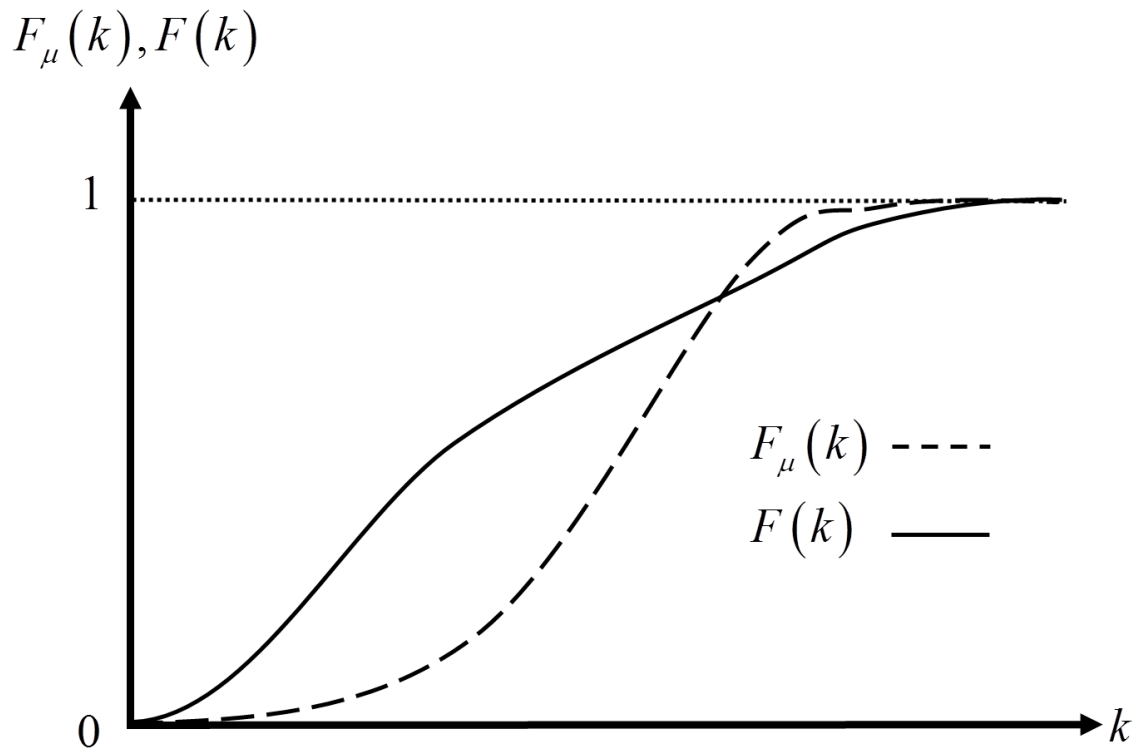


FIGURE 3. Functions F_μ and F are both increasing with respect to k .

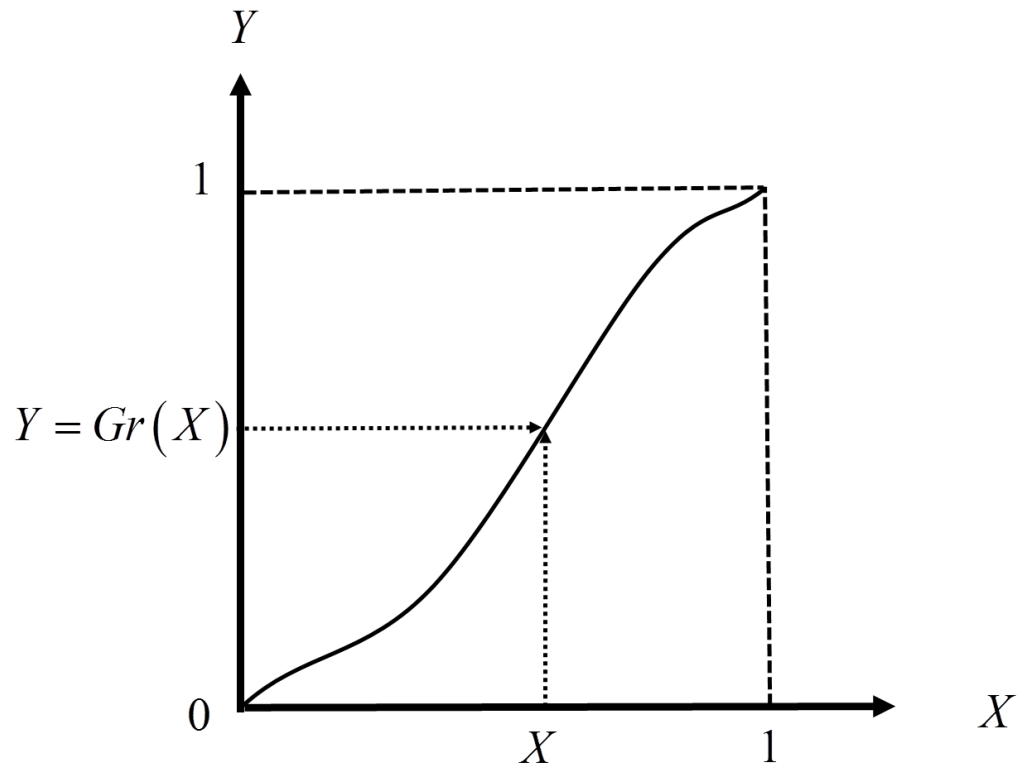


FIGURE 4. Visualization of definition of function Gr by Eq. (5), where the solid line is a

parametric curve given by equation $\begin{cases} X = F_{\mu}(k) \\ Y = F(k) \end{cases}, 0 < k < +\infty .$

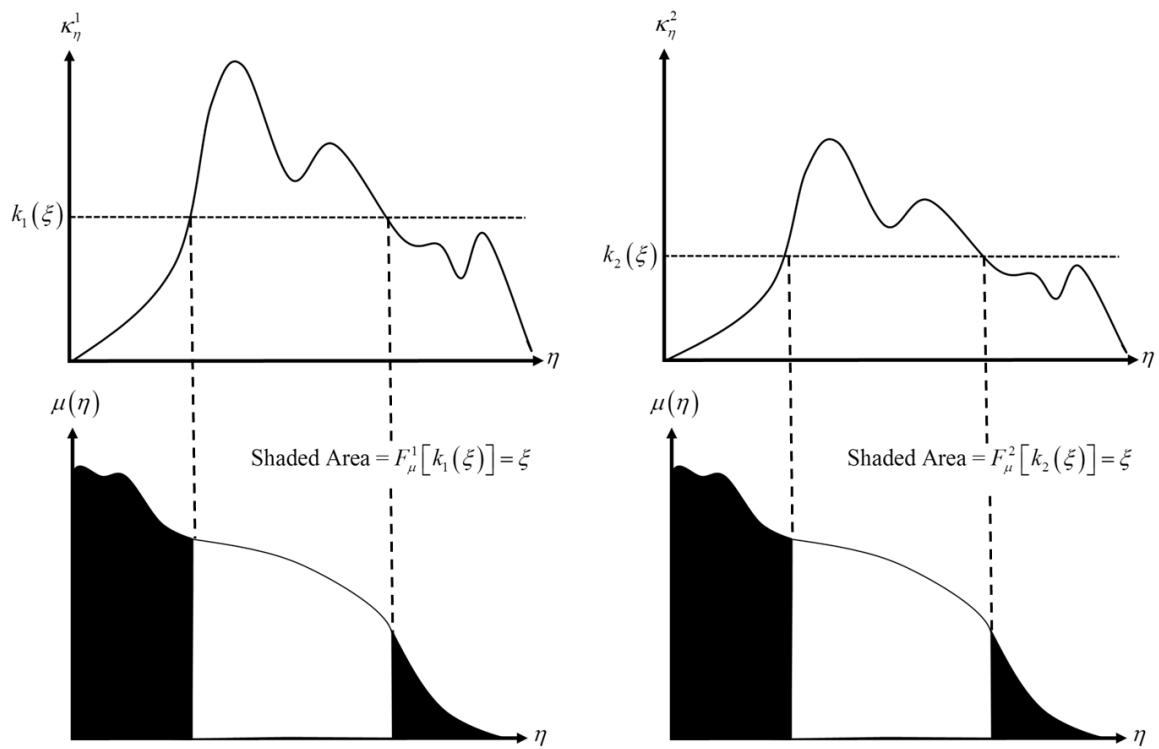


FIGURE 5. Comonotonicity: with arbitrary measure.

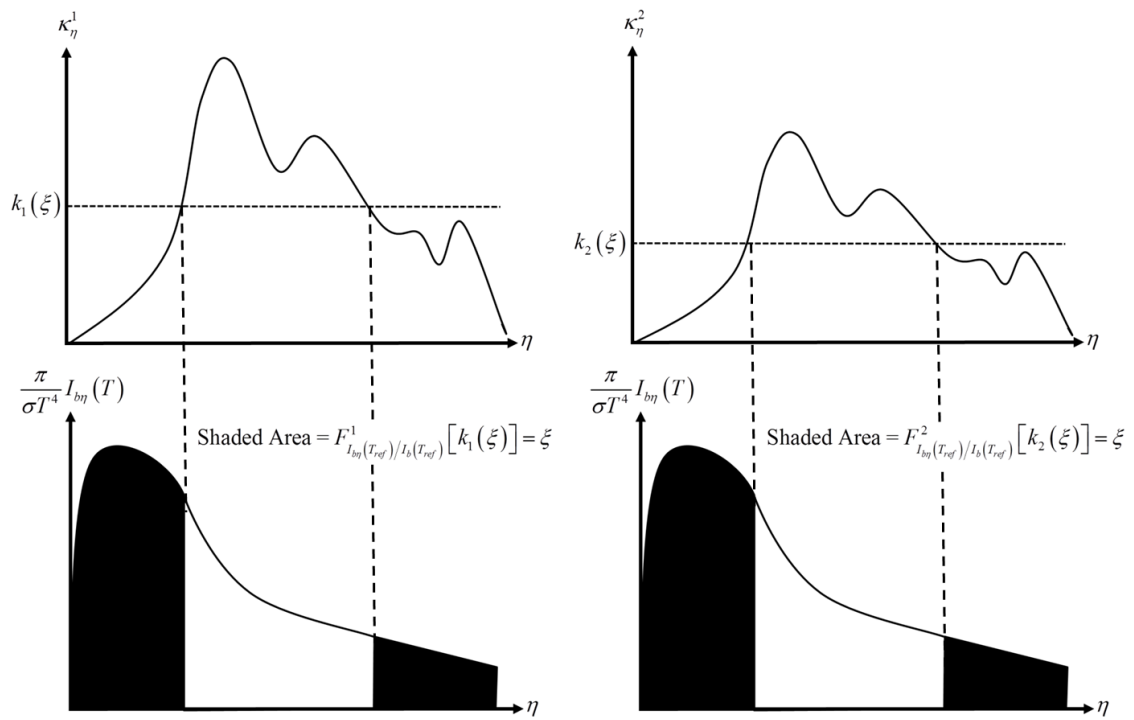


FIGURE 6. Comonotonicity: Rank Correlated Generalized SLW model [5] with measure

$$\mu(\eta) = \mu(\eta, T_{ref}) = I_{b\eta}(T_{ref}) / I_b(T_{ref}).$$

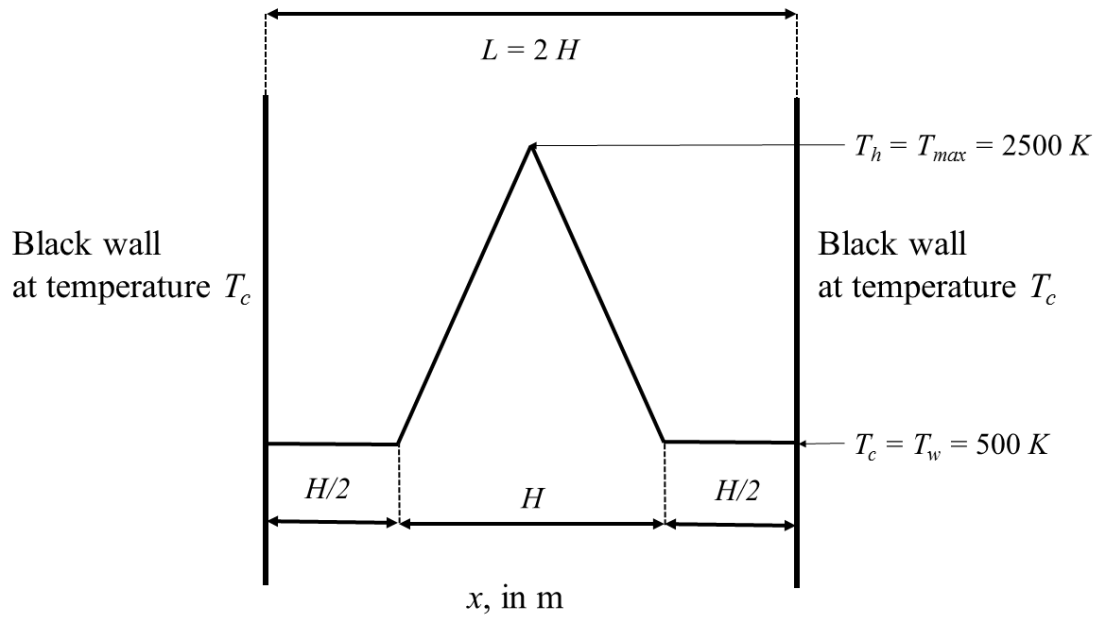


FIGURE 7. Triangular temperature profile considered for the comparison of the SLW model with the reference approach described in Ref. [2], RC-SLW model Ref. [5] and LBL calculations.

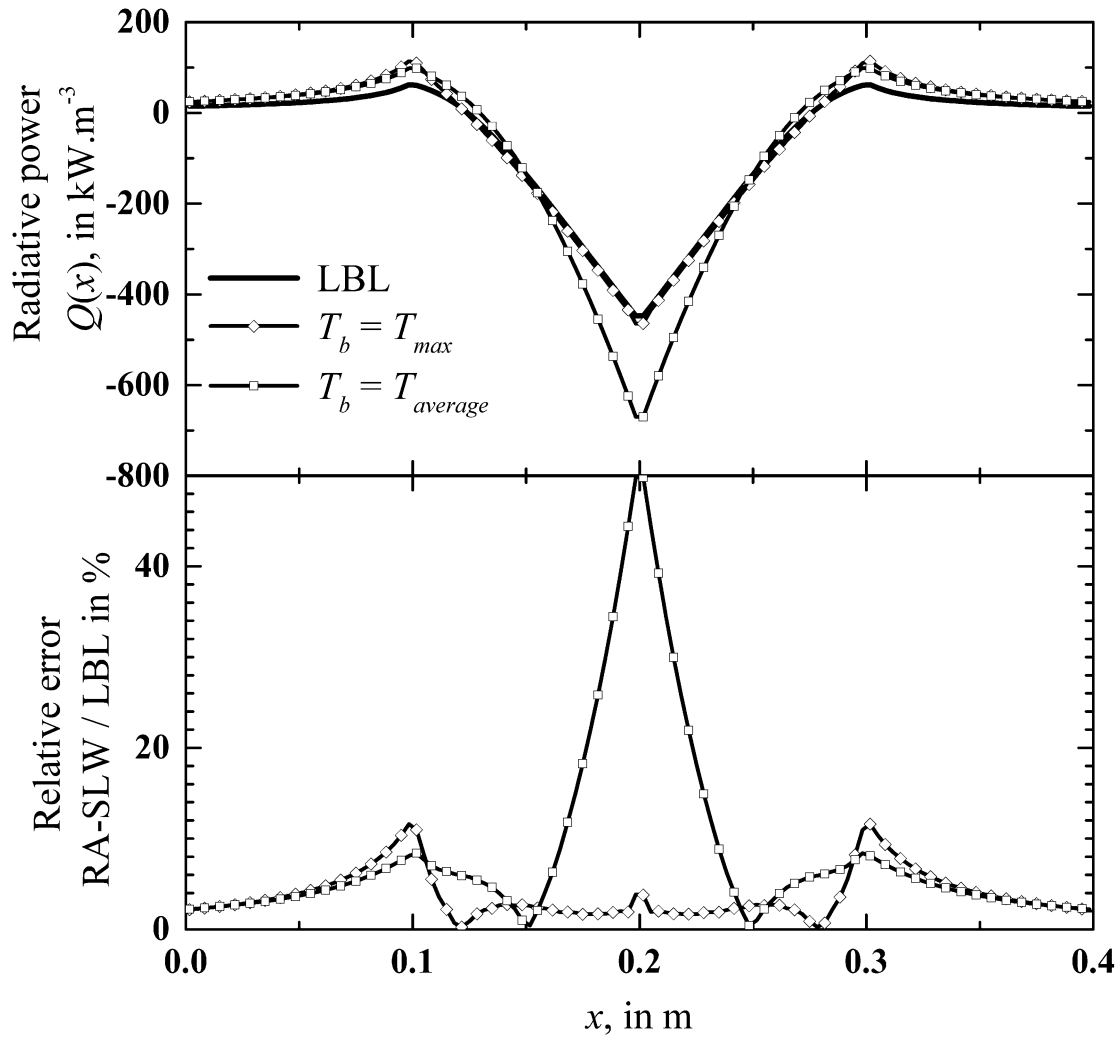


FIGURE 8. Comparison of the SLW model with the reference approach of Ref. [2] (RA-SLW) with LBL reference calculations. Triangular temperature profile of Figure 7; H₂O-N₂ mixture ($x_{\text{H}_2\text{O}} = 0.1$) at atmospheric pressure. Relative errors are calculated as

$$\frac{Q_{\text{LBL}}(x) - Q_{\text{RA-SLW}}(x)}{\text{Max}_{x \in [0, 2H]} |Q_{\text{LBL}}(x)|}.$$

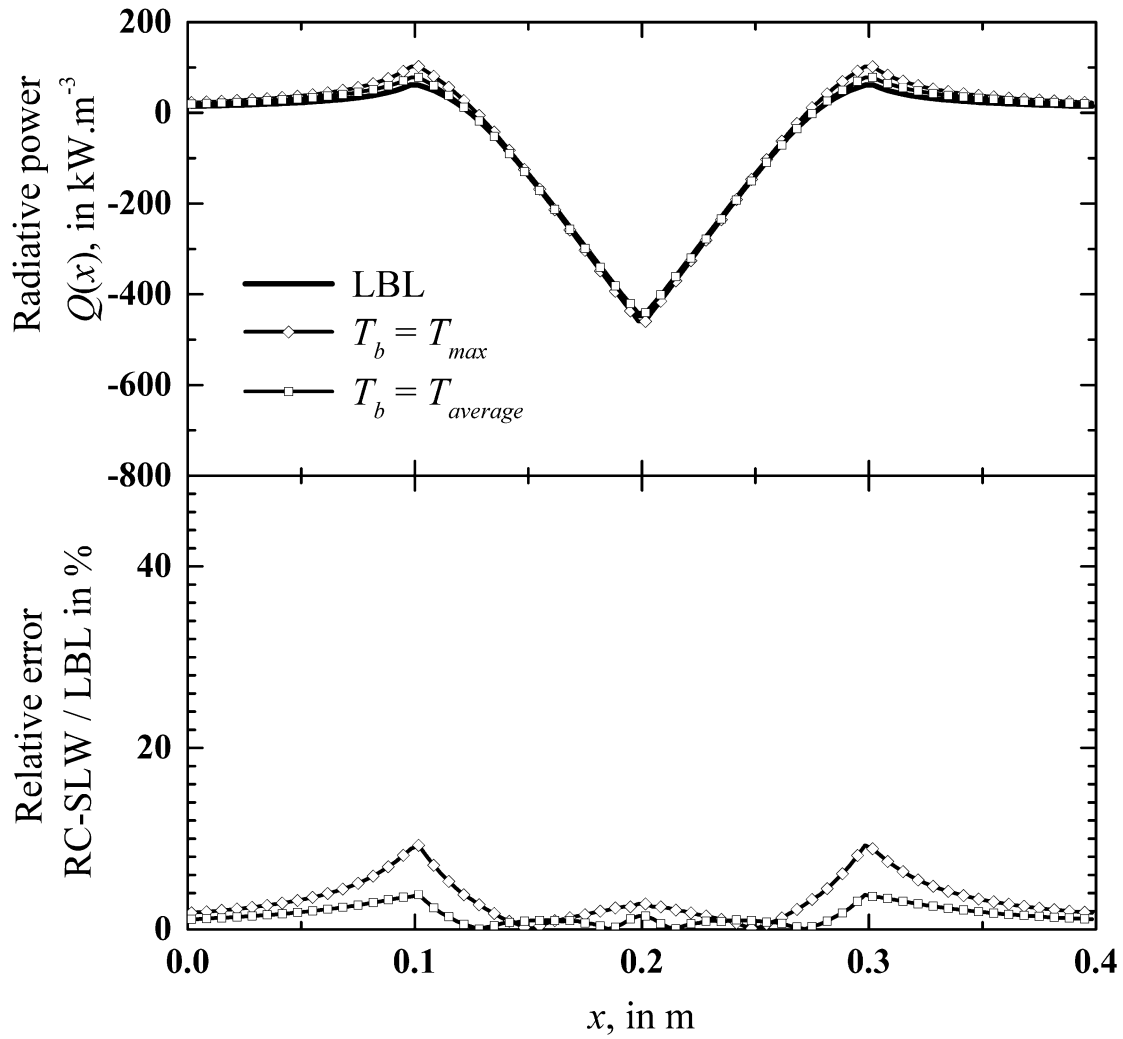


FIGURE 9. Comparison of the RC-SLW [5] model with LBL reference calculations.

Triangular temperature profile of Figure 7 ; H₂O-N₂ mixture ($x_{\text{H}_2\text{O}} = 0.1$) at atmospheric

pressure. $H = 0.2$ m. Relative errors are calculated as $\frac{Q_{\text{LBL}}(x) - Q_{\text{RC-SLW}}(x)}{\text{Max}_{x \in [0, 2H]} |Q_{\text{LBL}}(x)|}$.

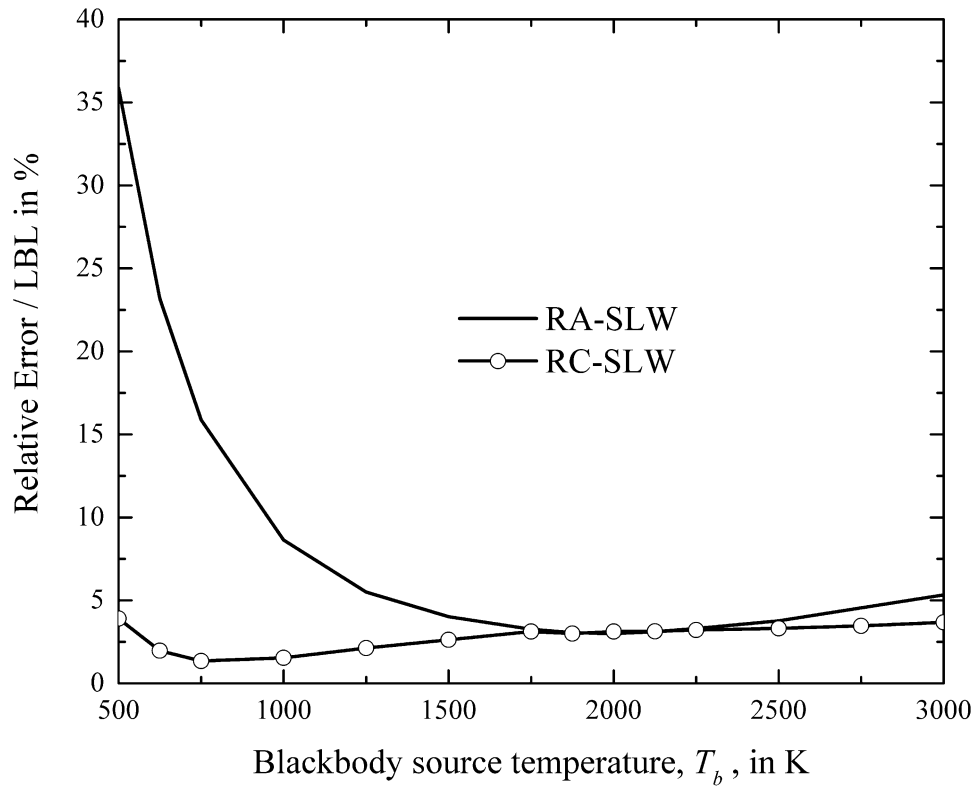


FIGURE 10. Relative errors of the RA-SLW and RC-SLW models for different blackbody source temperatures.