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Functional data analysis applied to the multi-spectral correlated–*k* distribution model

Longfeng Hou[a,b,*], Mathieu Galtier[b], Vincent Eymet[c,1], Frederic André[b], Mouna El Hafi[d]

[a] University of Shanghai for Science and Technology, School of Energy and Power Engineering, Shanghai, 200093, PR China
[b] Univ Lyon, CNRS, INSA-Lyon, Université Claude Bernard Lyon 1, CETHIL UMR5008, F-69621, Villeurbanne, France
[c] Méso-Star SAS, 8 rue des pêchers, 31410 Longages, France
[d] Université Fédérale de Toulouse Midi-Pyrénées, Mines Albi, UMR CNRS 5302, Centre RAPSODEE, Campus Jarlard, F-81013, Albi CT Cedex, France

ABSTRACT

The C*k* (Correlated-*k*) approach is among the most used method for the approximate modelling of the radiative properties of gases both in uniform and non-uniform media. One of its main defects is that the treatment of non-uniform gas paths is founded on the assumption of correlation - in fact co-monotonicity - of gas absorption coefficients in distinct states which is not rigorously verified for actual spectra. This correlation assumption fails as soon as large temperature gradients are encountered along the radiative path lengths. In order to circumvent this problem, a method based on functional data analysis (FDA) - referred to as the MSC*k* model in this work - was proposed in Refs. [1,2]. The principle of the method is to group together wavenumbers with respect to the spectral scaling functions - defined as the ratio between spectral absorption coefficients in distinct states - so that the correlation/co-monotonicity assumption can be considered as exact over the corresponding intervals of wavenumbers. Very few details were provided up to now about the application of FDA within the frame of the MSC*k* model. Indeed, most of our previous works were dedicated to the derivation of the methods itself. Accordingly, in the present paper, we mostly focus our attention on the mathematical definition of clusters of scaling function, quantities which are used to build spectral intervals over which gas spectra in distinct states are assumed to be scaled. The comparison of different clustering methods together with the criterion to select an appropriate number of clusters are described and discussed and the application of this approach for several test cases, including 3D geometries, are presented.

1. Introduction

Radiative heat transfer in gaseous media plays a key role in a wide range of industrial applications: high temperature combustion chambers [3], gas turbine combustors [4], long-range IR sensing [5], fire safety [6], *etc*.

In all these applications, evaluating the radiative heat transfer inside the gaseous medium requires modelling its radiative properties over any possible gas path. Among the models available in the literature, the C*k* approach is one of the most popular. Its extension in the narrow band (NBC*k*), full spectrum (FSC*k*) and the statistical narrow band version (SNBC*k*) has been discussed by Chu [7] and Consalvi [8]. Chu [7] found that the SNBC*k* is sufficiently accurate to generate benchmark results for multi-dimensional radiation problems. Consalvi [8] compared several usual radiation models and concluded that NBC*k* model provides accurate results in the case of axisymmetric pool fires.

However, the main theoretical defect of the C*k* model for applications in non-uniform media is that band intervals are treated as a whole, without any verification of the correlation assumption. This leads to the breakdown of the assumption of rank correlation of gas spectra in distinct states when large temperature gradients exist in the medium studied [9]. In order to circumvent this problem, we introduced a method based on functional data analysis (FDA) [10] and called the MSC*k* model [1,2]. The main ideas behind the MSC*k* approach are not new, as they share similar concepts as used in mapping methods such as described in West and Crisp [11] or in the multiscale method of Zhang [12]. The objective of this method is in fact to group together wavenumbers according to the spectral scaling functions [1] defined as the ratio between spectra in different thermophysical states. Over these intervals, the correlation assumption can be considered as exact. It has already been shown that the MSC*k* model with 25 clusters, defined over a narrow band (25 cm^{-1}), is more accurate than the medium resolution

* Corresponding author. University of Shanghai for Science and Technology, School of Energy and Power Engineering, Shanghai, 200093, PR China.
E-mail address: longfenghou@126.com (L. Hou).
[1] www.meso-star.com.

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(1 cm^{-1}) C*k* model when compared with LBL benchmark calculations at nearly the same computational cost [2]. Meanwhile, the MSC*k* model has almost the same accuracy as the CKFG (Correlated-k Fictitious Gas) [13] technique in infrared signature cases, but at lower computational costs [14]. Another advantage of the MSC*k* model, compared to CKFG, is that MSC*k* can be applied in the case of reflecting walls, which is not compatible with the CKFG model which requires a formulation in terms of transmissivities [2].

The concept of clusters is one of the most important in the building of MSC*k* model coefficients. In this paper, we mostly focus our attention on the basic mathematical definition of clusters of scaling functions and on the comparison of different clustering methods. The definition of clusters of scaling functions is given in Section 2. Comparisons between different clustering methods are discussed in detail in Section 3 and the arbitrary choice of the number of clusters is addressed in Section 4. Application of the proposed model for current radiative heat transfer calculations is provided in Section 5.

2. Clustering scaling functions

2.1. Correlation assumption

In the C*k* model, the assumption of co-monotonicity - *viz.* the preservation of the ranks between spectra in distinct states, originally referred to as rank correlation in Ref. [15] in which this idea was first introduced - is used to extend the *k*-distribution method from uniform to non-uniform gas paths. The aim of this subsection is to discuss the physical reasons that explain why the correlation assumption is likely to fail in media with high temperature gradients.

The correlation/co-monotonicity assumption can be formulated as follows: for any wavenumber η inside a narrowband $\Delta\eta$, the absorption coefficient $\kappa_\eta(\underline{\phi})$ at thermophysical condition $\underline{\phi}$ can be represented as a function H (strictly monotonic, and more precisely increasing) of $\kappa_\eta(\underline{\phi}^{ref})$, as:

$$\kappa_\eta(\underline{\phi}) = H[\kappa_\eta(\underline{\phi}^{ref})] \tag{1}$$

where $\kappa_\eta(\underline{\phi}^{ref})$ is the absorption coefficient at the same wavenumber in some prescribed reference thermophysical condition $\underline{\phi}^{ref}$. As H is strictly increasing by assumption, $\kappa_\eta(\underline{\phi})$ and $\kappa_\eta(\underline{\phi}^{ref})$ share the same monotonicity: this means that for any couple of wavenumbers η_1 and η_2, if we have $\kappa_{\eta_1}(\underline{\phi}^{ref}) > \kappa_{\eta_2}(\underline{\phi}^{ref})$ in the reference state, then we can draw the conclusion that $\kappa_{\eta_1}(\underline{\phi}) > \kappa_{\eta_2}(\underline{\phi})$ in state $\underline{\phi}$ at the same spectral location.

This assumption is accurate as soon as temperature gradients are small along non-uniform paths. This explains why the C*k* method has encountered a great success to treat situations which involve small temperature gradients, such as encountered in atmospheric applications [16] [17] or radiative heat transfer in combustion chambers. However, for non-uniform media with large temperature gradients (such as encountered in remote sensing problems), the correlation assumption between gas absorption coefficients at different temperatures poorly represents the true behavior of gas spectra in distinct thermophysical states. This is mainly due to the appearance of so-called “hot lines” [13] that breaks the one-to-one correspondence between gas spectra assumed in Eq. (1).

A solution to this problem consists in building groups of wavenumber in such a way that the scaling function, defined as the ratio between the absorption coefficients in state $\underline{\phi}$ and in the reference thermophysical condition $\underline{\phi}^{ref}$, is uniform inside each of these groups. Built this way, gas spectra are scaled (linearly correlated, on can find more details in Page 321 of Ref. [7]) over the groups, which means that the assumption of co-monotonicity becomes, if not rigorous in practice, at least more relevant over the groups than over the whole band. This is the principle of many methods to improve gas radiation models in non-uniform media such as the multi-scale model by Modest and Zhang or the multi-spectral technique described in the present paper. Both of these methods are however funded on the same concept of mapping introduced in 1992 by West and Crisp within the frame of radiative heat transfer in non-uniform atmospheres [11].

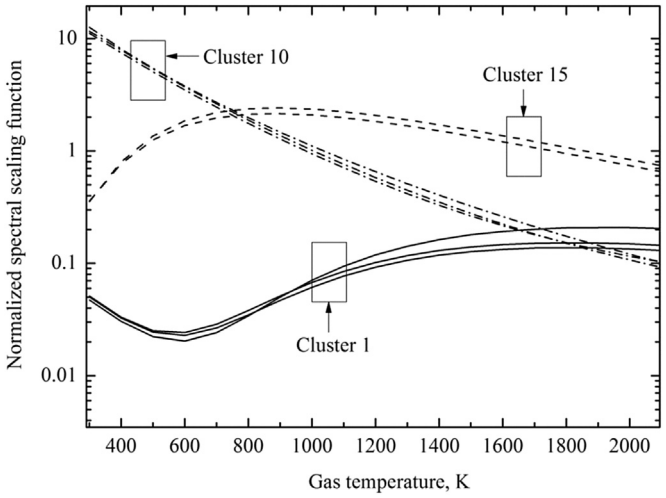

Fig. 1. Example of clusters for the [1487.5 cm^{-1}, 1512.5 cm^{-1}] spectral interval: 10% H_2O + 90% N_2.

Fig. 1 (inspired from Fig. 4 of Ref. [2]) depicts the results obtained by application of the clustering method to a narrow band [1487.5 cm^{-1}, 1512.5 cm^{-1}] of H_2O. Each of the curves corresponds to the variations of absorption coefficients as a function of the gas temperature. As shown in this figure, different clusters are associated with distinct behaviors of the absorption coefficient with respect to the gas temperature. At the same time, curves associated with wavenumbers inside the same clusters show very similar trends.

Building the spectral groups associated with similar scaling functions can be done using clustering techniques. But as the quantities to assemble are functions, specific techniques are required. They are usually referred to as Functional Data Analysis (FDA). These methods involve two distinct steps: 1/the first one is to propose a functional form to describe the data, 2/the second one is to apply standard clustering methods using grouping criteria defined in terms of integrals. These two aspects of the technique are described in the following sections.

2.2. Physical model of spectral scaling functions and similarity coefficient

The main difficulty for the application of FDA methods is to provide accurate approximations for the functions to group into clusters. The results provided in this subsection for the construction of scaling functions were described in Ref. [1]. Here, we only remind the final formulation for the completeness of the present work.

The scaling function is defined as the ratio between spectra in different thermophysical states:

$$u_\eta(\underline{\phi}) = \kappa_\eta(\underline{\phi})/\kappa_\eta(\underline{\phi}^{ref}) \tag{2.a}$$

In a series of discrete spectral data $\kappa_\eta(T_1), \cdots, \kappa_\eta(T_{n'})$, with $T_1 < T_2 < \cdots < T_{n'}$, the scaling function $u_\eta(T)$ (we restricted to the dependency with respect to temperature only) at T_1, T_2, ..., $T_{n'}$ can be obtained directly from Eq. (2.a) with n' pairs of ($\kappa_\eta(T_i)$, T_i).

For any temperature T such that $T_i < T < T_{i+1}$, we have the following approximation (this formulation is restricted to the dependency with respect to temperature):

$$\kappa_\eta(T) = \kappa_\eta(T_i)\exp\left[\int_{T_i}^{T} \frac{\partial ln\, u_\eta(T')}{\partial T'} dT'\right] \approx \kappa_\eta(T_i)\exp\left[\frac{T - T_i}{T_{i+1} - T_i} ln\frac{u_\eta(T_{i+1})}{u_\eta(T_i)}\right] \tag{2.b}$$