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On the use of polynomial chaos expansions and generalized moments within the frame of gas radiation in non-uniform media

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ABSTRACT

In many applications involving gaseous media at high temperature, accurate but computationally efficient models are required for the radiative properties of gases. The aim of the present work is to show how, by combining results from Polynomial Chaos framework and Devyatov's Method Of Moments, one can provide simple estimates of the transmission functions of gases both in uniform and non-uniform media. The proposed model only involves polynomials. It is probably one of the simplest in terms of mathematical formulation but also one of the most sophisticated, considering the concepts that it involves. It can be applied in uniform and non-uniform media, where it is shown to be equivalent, in terms of accuracy, to usual C–*k* models.

1. Introduction

Radiative heat transfer in gaseous media arises in many situations. Gases may be at high temperature, as in combustion applications, or cold, as in some atmospheric studies. The most accurate model to estimate the radiative properties of gases is the so-called Line-By-Line (LBL) approach [1,2]. It consists in calculating gas absorption spectra at high resolution directly from spectroscopic databases. Nevertheless, it is too computationally expensive to be considered in many cases (such as in multi-physic or three-dimensional problems) for which more computationally efficient approaches are required.

Many approximate models were proposed during the past decades. Most of them (especially those based on the so-called *k*-distribution approach, [3]) achieve LBL accuracy in uniform situations. Usually, their main source of error comes from the approximate treatment of non-uniformities that requires additional assumptions, such as the scaling or correlation of absorption spectra in various thermophysical states. In most situations, those assumptions provide accurate results, as soon as small temperature gradients are found inside the gas. When higher gradients are involved, recourse to more sophisticated techniques, such as the Multi-Group [4,5], Fictitious gases [6] or Multi-spectral [7,8] approximations, is required.

Recently, the generalized *k*-moment approach [9,10] was proposed to estimate cumulative distribution functions directly from LBL data. The method enables to represent those functions as sums of polynomials of a certain type: the so-called Cutteridge–Devyatov polynomials. It was found to be accurate both for the calculation of distribution functions and for applications in radiative heat transfer (results, in terms of narrow band averaged spectra, are provided in the case of H_2O in Ref. [10]).

The Generalized *k*-moment approach is based on Devyatov's Method of Moments (DMM) described in Refs. [11,12]. This method is similar to the so-called Polynomial Chaos (PC) technique proposed in 1938 by Wiener [13], but

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introduced in a slightly different way. Some theoretical links between the two approaches are discussed in this paper (additional details are also provided in Appendix A).

The aim of the present work is to show how, by combining results from PC and DMM, it is possible to propose simple and accurate models for the radiative properties of gases in uniform and non-uniform media. It is organized as follows: in Section 2, the method is introduced by considering the problem of estimating a scaling function between spectra in two distinct thermophysical states; Section 3 is dedicated to a short description of the PC framework; in Section 4, it is shown how it is possible to replace the implicit equation associated to the scaling assumption, which is highly nonlinear, by a simple polynomial one from the use of concepts taken from PC theory. Explicit formulae are also given to estimate transmission spectra as polynomials; Sections 5 describe some results of comparisons of the proposed Cutteridge–Devyatov Polynomial Chaos (CDPC) model and reference Line-By-Line calculations. CDPC approximation is shown to provide results as accurate as usual k-distribution approaches at a very low computational cost (polynomials at orders 10–14) in uniform and non-uniform situations.

2. Principle of the method

In order to introduce our methodology, we are going to study the following problem. We consider a spectral band $\Delta\eta$ over which: (1) the Planck function is constant (we thus restrict here our approach to narrow band models), (2) the absorption coefficient in any thermophysical state takes strictly positive values (no transparency region of the gas is inside the interval). We define a reference length that will be from now on written L^{ref} and two thermophysical states. They are represented as vectors $\underline{\phi}$ whose components are the temperature, total pressure and composition of the gas associated to each state. One of them will be written $\underline{\phi}^{ref}$, and will play the role of a reference, and the second one $\underline{\phi}$. Gas spectra are assumed to be scaled (as defined by Modest in Ref. [3] – see Eq. (30) from this reference) which means that we can find a real u, that depends implicitly on the state vectors $\underline{\phi}^{ref}$ and $\underline{\phi}$ such that

$$\frac{1}{\Delta\eta}\cdot\int_{\Delta\eta}\exp\left[-\kappa_\eta\left(\underline{\phi}\right)\cdot L^{ref}\right]d\eta=\frac{1}{\Delta\eta}\cdot\int_{\Delta\eta}\exp\left[-u\cdot\kappa_\eta\left(\underline{\phi}^{ref}\right)\cdot L^{ref}\right]d\eta \tag{1}$$

Our objective is to find u.

Let us assume that the solution u to Eq. (1) lies inside some bounded interval, $[u_{\min},u_{\max}]$ with $u_{\max}>u_{\min}>0$ (this obviously restricts the approach to spectral bands over which the gas is not transparent, as assumed previously). If we have no a priori information about the solution, then the range $[u_{\min},u_{\max}]$ extends over several orders of magnitude (due to the behavior of absorption spectra). Accordingly, we normalize the search space over which we are going to seek u by introducing a new variable, that will be written ξ, such that

$$u=u(\xi)=u_{\min}\cdot\left(\frac{u_{\max}}{u_{\min}}\right)^{\xi},\quad \xi\in[0,1] \tag{2}$$

In order to introduce the concept of Polynomial Chaos in a simple way, let us describe how the problem set by Eq. (1) could be handled by application of a Stochastic Optimization Technique. Using this kind of methods to solve Eq. (1) would consist of the following steps [14]:

1. for a prescribed integer number N, choose inside the interval $[0,1]$ N random numbers $\xi_1,\ldots,\xi_N$ according to a uniform probability distribution. Then, the objective function $F(\xi)$ defined as (from Eq. (1))

$$\begin{aligned}F(\xi)&=\frac{1}{\Delta\eta}\cdot\int_{\Delta\eta}\exp\left[-u(\xi)\cdot\kappa_\eta\left(\underline{\phi}^{ref}\right)\cdot L^{ref}\right]d\eta\\&\quad-\frac{1}{\Delta\eta}\cdot\int_{\Delta\eta}\exp\left[-\kappa_\eta\left(\underline{\phi}\right)\cdot L^{ref}\right]d\eta\\&=\tau^{\Delta\eta}\left[L(\xi),\underline{\phi}^{ref}\right]-\tau^{\Delta\eta}\left(L^{ref},\underline{\phi}\right)\end{aligned} \tag{3a}$$

   where

$$\tau^{\Delta\eta}\left[L(\xi),\underline{\phi}^{ref}\right]=\frac{1}{\Delta\eta}\cdot\int_{\Delta\eta}\exp\left[-\kappa_\eta\left(\underline{\phi}^{ref}\right)\cdot\underbrace{u(\xi)\cdot L^{ref}}_{L(\xi)}\right]d\eta \tag{3b}$$

   and

$$\tau^{\Delta\eta}\left(L^{ref},\underline{\phi}\right)=\frac{1}{\Delta\eta}\cdot\int_{\Delta\eta}\exp\left[-\kappa_\eta\left(\underline{\phi}\right)\cdot L^{ref}\right]d\eta \tag{3c}$$

   can be evaluated to provide N values of F: $F(\xi_1),\ldots,F(\xi_N)$.
2. The next step is usually to search the integer index $i\in\{1,\ldots,N\}$ that corresponds to the minimum of the absolute value of $F(\xi_i)$, $\xi_i\in\{\xi_1,\ldots,\xi_N\}$. This index is associated to the best estimate, inside the set $\{\xi_1,\ldots,\xi_N\}$, of the solution to Eq. (1).
3. If the value of $F(\xi_i)$ is lower than a user-defined threshold, then stop the process. Otherwise, apply the evolutionary process associated to the chosen Stochastic Optimization Technique (by combining/mutating genes in the case of Genetic Algorithms, or by generating a direction of propagation for Particle Swarm techniques, etc) and go back to step 1.

The task of the evolutionary scheme is to decrease, at each step of the process, the size of the search space. The method is thus iterative and continues until the algorithm finds a value $F(\xi_i)$ that is below the prescribed threshold, or if a maximum number of iterations is reached. Clearly, this approach may be computationally expensive in a general frame.

One possible way to reduce the computational cost required to minimize function F is to use the set of estimates obtained at the end of the first iteration, viz. $F(\xi_1),\ldots,F(\xi_N)$, and approximate the whole function F by using a surrogate model. The simplest choice to handle this problem is by fitting the set of data $F(\xi_1),\ldots,F(\xi_N)$ by a polynomial $P(\xi)$ at an order $M\leq N$. The mathematical problem then consists in finding the coefficients $\{p_0,p_1,\ldots,p_M\}$ of the polynomial $P(\xi)=p_0+p_1\cdot\xi+\cdots+p_M\cdot\xi^M$ that minimize the following sum of squares:

$$\sum_{n=1}^{N}\left[P(\xi_n)-F(\xi_n)\right]^2 \tag{4}$$