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## Comparison of three spatial differencing schemes in discrete ordinates method using three-dimensional unstructured meshes

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#### Abstract

A radiative heat transfer code based on the discrete ordinates method applied to unstructured grids has been developed to be coupled with a finite volume CFD code for combustion applications. The constraints are that: (1) Accurate coupling with a finite volume CFD code requires that the output is the integrated radiative source term within each mesh; (2) The resulting computation times must remain acceptable within the combustion requirements (of the order of an hour for realistic industrial geometries); (3) the line spectra of combustion gases must be accurately represented across the whole infrared range. Here, gaseous line spectra properties are represented with the SNB-*ck* model using narrow bands parallelization. The radiative transfer equation is discretized with a finite volume approach and three schemes are tested ("exponential", "step" and "diamond mean flux") in terms of accuracy and computational requirement. They are first tested for academic gray cases, solutions being compared to reference solutions provided by the Ray Tracing Method and the Monte Carlo Method. The behavior of the three schemes is also discussed for a spherical geometry, using an analytical solution in order to perform a parametric study of the absorption optical thickness influence in a wide range typical of spectral line gaseous radiation. Final tests involving a complete water vapor spectrum are performed in order to test the effects of preceding conclusions in terms of expected accuracies for combustion applications. © 2005 Elsevier SAS. All rights reserved.

Keywords: Radiative transfer; Infrared line spectra; Discrete ordinates; Unstructured grids; Three-dimensional

### 1. Introduction

In computational fluid dynamics (CFD), the coupling between radiative heat transfer and combustion is based on the resolution of the energy equation. The heat source term due to radiation is evaluated by taking into account the temperature and radiating species concentration profiles, which are obtained from the solution of the aerothermochemistry equations. Among all the numerical methods developed to calculate the radiative heat transfer, the finite volume method (FVM) and the discrete ordinates method (DOM) offer good compromises between accuracy and computational requirements. These approaches have been widely used to solve radiative transfer problems in structured three-dimensional geometries using Cartesian or cylindrical coordinates. In particular, the DOM, described by Chandrasekhar in 1950 [1], has been deeply studied by Lathrop and Carlson in 60-70's [2] and by Truelove, Fiveland and Jamaluddin in the 80's [3–7]. Significant improvements have been achieved in the last decade aiming at the reduction of the ray effects and false scattering, more accurate quadratures and the extension to complex geometries. Nevertheless, the coupling between radiative transfer and other physical phenomena, such as combustion and fluid flow at high temperatures, requires the solution of the radiative transfer equation using the same grid employed to solve the other governing equations.

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### Nomenclature

Α	surface area m <sup>2</sup>
$A_{\Delta}$	surface area of cell orthogonally planned
	following $\mathbf{s}_i$ $m^2$
$D_{ij}$	scalar product of $\mathbf{s}_i$ by $\mathbf{n}_j$
G	incident radiation $\dots W \cdot m^{-2}$
Ι	radiation intensity $W \cdot m^{-2} \cdot sr$
$N_{\rm dir}$	number of discrete directions
$N_{\rm face}$	number of faces of cells
$Q_w$	net heat flux at the wall $\dots W \cdot m^{-2}$
R	radius m
$S_r$	radiative source term $\dots W \cdot m^{-3}$
Т	temperature K
V	volume m <sup>3</sup>
$\overline{I_{\text{in}}}$	averaged intensity over entries $\dots$ W·m <sup>-2</sup> ·sr
<i>I</i> <sub>out</sub>	averaged intensity over exit faces $W \cdot m^{-2} \cdot sr$
$\mathbf{Q}_r$	radiative heat flux vector $\dots W \cdot m^{-2}$
n	unit vector normal to the face
S	discrete direction unit vector
$f_v$	soot volumetric fraction
h	height m
$l_{max}$	maximum thickness of a cell m
S	coordinate along direction s
t	optical pathlength through a cell m

Unstructured grids are often used in CFD owing to their geometrical flexibility. In this way, a lot of work has been developed during the last decade to apply the DOM-FVM to non-orthogonal structured grids and unstructured grids in three-dimensional enclosures [8-11,15]. In particular, Sakami and co-workers proposed an accurate method for the spatial discretization by taking into account the exponential extinction [12-14], but it necessitates to perform a heavy preprocessing procedure. Much less sophisticated schemes are also commonly used. Liu et al. [15] have used the "step" scheme, equivalent of the "upwind" scheme in CFD and Ströhle et al. [17] have proposed the mean flux interpolation scheme. Another type of spatial discretization was also recently introduced, namely the Discrete Ordinates Interpolation Method (DOIM), which does not rely upon an integration of the radiative transfer equation over the control volumes, but rather on the integration of the equation along a line of sight. This method has been introduced by Seo et al. in 1998 [18] and extended to unstructured grids by Cha et al. in 2000 [19]. Lastly, Koo et al. [20] have compared three methods applied to two-dimensional curved geometries: the DOIM, Sakami's approach and the discrete ordinates method in orthogonal curvilinear coordinates [21].

In our study, a computer code using unstructured meshes and based on the modeling of radiative transfer using the DOM has been developed aiming at a future coupling with a

w	weight associated to a discrete direction	
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Greek symbols		
α	weighting factor for mean flux scheme	
ε	emissivity	
κ	absorption coefficient $\dots \dots \dots$	
μ, η, ξ	director cosines of the discrete direction	
ν	wave number $\dots m^{-1}$	
${\Sigma}$	surface area delimiting a volume $\dots m^2$	
τ	absorption optical thickness	
$\Omega$	solid angle sr	
Subscripts		
А	beginning point of a pathway through a cell	
В	ending point of a pathway through a cell	
b	blackbody	
i	associated to <i>i</i> th discrete direction of the	
	angular quadrature	
j	associated to <i>j</i> th face of the cell	
k	associated to kth entry of the cell	
l	associated to <i>l</i> th exit face of the cell	
Р	associated to the volume of the cell	
w	wall	
x, y, z	Cartesian coordinates	
, , , , .		

combustion finite volume code available at the CERFACS<sup>1</sup> in France. The code has been specially written for unstructured grids using tetrahedrical cells, by trying to avoid complex adaptations that are highly time consuming. The constraints associated to combustion applications where the following:

- Accurate coupling with a finite volume CFD code requires that the output is the integrated radiative source within each mesh;
- (2) The resulting computation time must remain acceptable for realistic industrial geometries in combustion;
- (3) The line spectra of combustion gases must be accurately represented across the whole infrared range.

Then, to treat general combustion situations, even if the main part of this paper is devoted to gray media, all these constraints lead to the following choices:

 Gaseous line spectra properties are represented with a Statistical Narrow Band *correlated-k* model and parallelization is used to simultaneously compute the radiative contribution of each narrow band;

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