

# Evaluation of flame emission models combined with the discrete transfer method for combustion system simulation

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## Abstract

This article considers the application of flame emission models used for predicting the thermal radiation fluxes from flames and fires within a computational fluid dynamic framework, used in conjunction with the discrete transfer method. The flame emission models differ in their generality, sophistication, accuracy and computational cost, and are assessed in terms of their ability to predict radiation transfer in idealised situations, as well as flames in tubes representative of burner systems, laboratory-scale jet flames and wind-blown jet fires. It is concluded that the implementation of simple flame emission models, based on the grey gas assumption, must be treated with caution due to convergence problems. The key problem occurs when the grey absorption coefficient is based on a length scale linked to the size of the control volume. This issue is well known in the radiation modelling community, but not so in the combustion modelling community. Use of models based on the banded mixed grey gas, TTNH, wide and narrow band approaches yield satisfactory results for all the simulated flames and fires considered, typically being within 20% of the measured radiation heat flux.

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## 1. Introduction

The mathematical modelling of high temperature processes requires an ability to predict the thermal radiation fields with confidence. The fundamental quantity of interest, the spectral intensity, depends in a complex way on the temperature and participating species distributions. This, together with the fact that the spectral

intensity is a function of location, orientation and wavelength, makes the simulation of combusting flows a challenging scientific computation. Even with today's computer hardware and the routine use of parallel computing facilities choices have to be made regarding the balance between the levels of sophistication of the radiation model relative to other sub-models that form the composite flame or fire model. In this article a number of radiation models are evaluated with respect to their accuracy and suitability to be combined with a computational fluid dynamic (CFD) model for simulating a number of idealised and generic flows.

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## Nomenclature

|                        |  |
|------------------------|--|
| $a_{i,j,1}, a_{i,j,2}$ | coefficients in the mixed grey gas model                           |
| $f_v$                  | soot volume fraction   |
| $I$                    | spectrally integrated intensity                                    |
| $I_{b,v}$              | black body spectral intensity                                      |
| $k$                    | wall thermal conductivity  |
| $K_a$                  | grey gas absorption coefficient                                    |
| $l$                    | path length  |
| $n$                    | number of control volumes  |
| $N_\varphi$            | number of rays in the $\varphi$ direction                          |
| $N_\theta$             | number of rays in the $\theta$ direction                           |
| $N_{\text{Ray}}$       | number of rays   |
| $N_g$                  | number of grey gases for gas emission in the mixed grey gas model  |
| $N_s$                  | number of grey gases for soot emission in the mixed grey gas model |
| $q$                    | heat flux  |
| $q_{\text{tot}}$       | total heat flux  |
| $q_{\text{CD}}$        | conduction heat flux through wall                                  |
| $q_{\text{CV}}$        | convection heat flux to wall                                       |
| $q_{\text{R}}$         | radiation heat flux  |
| $r$                    | radial distance  |
| $S$                    | speed-up factor  |
| $S_{\text{CV}}$        | speed-up factor per control volume                                 |
| $S_{\text{Ray}}$       | speed-up factor per ray  |
| $S/d$                  | mean line intensity to line spacing ratio                          |
| $T$                    | temperature  |
| $T_{\text{water}}$     | cooling water temperature  |
| $x$                    | downwind distance or axial distance                                |
| $X_j$                  | partial density path length of species $j$                         |

## Greek symbols

|                          |  |
|--------------------------|--|
| $\alpha$                 | integrated band intensity                |
| $\Delta s$               | path length through a homogeneous volume |
| $\Delta_w$               | wall thickness                           |
| $\varepsilon_{\text{T}}$ | total emissivity                         |
| $\varepsilon_w$          | wall emissivity                          |
| $\eta$                   | line width to spacing ratio              |
| $\varphi$                | angle of rotation                        |
| $\nu$                    | wave number                              |
| $\nu_u$                  | upper limit on a wide band               |
| $\theta$                 | angle of incidence                       |
| $\rho$                   | partial density                          |
| $\sigma$                 | Stefan Boltzmann constant                |
| $\tau$                   | transmittance                            |
| $\tau_{\text{H}}$        | optical depth at band head               |
| $\omega$                 | band width parameter                     |

## Subscripts

|            |  |
|------------|--|
| –          | property incident to a wall                      |
| +          | property emitted from wall                       |
| g          | gas phase property                               |
| $i$        | spectral band                                    |
| $i, j$     | ray indices                                      |
| $j$        | gaseous species                                  |
| $n, n - 1$ | exit and entry points of ray traversing a volume |
| $\nu$      | spectral property                                |
| s          | property of soot                                 |
| w          | wall property                                    |

Example areas of application are as part of mathematical models used in the safety analysis of high-pressure plant and pollution control in heating plant. The safe design and operation of high-pressure plant and pipe work requires that provision be made for the relief of pressure under certain operational and emergency conditions. The consequences of a release must also be evaluated so that appropriate safety measures can be adopted during the relief process. In addition, assessments of the consequences associated with accidental releases of flammable material are required as the basis of safety reports and risk assessments on existing and proposed installations. For flammable gases and vapours it is necessary to be able to predict the thermal radiation fluxes that any fire might impose on its surroundings—either by direct flame impingement of the fire on an item of plant or at distance from the fire by radiation transmitted through the atmosphere. This information is in turn used to provide estimates, for example, of vessel survival times, building burning distances and escape times for personnel.

In addition to the safety analysis of fires, increasing concerns over the environmental impact of heating plant such as boilers and furnaces requires that the energy balance during their operation is evaluated accurately. Insight into the energy transfer processes of heating plant is necessary to ensure that the temperature sensitive reaction rates relevant to pollution production, such as  $\text{NO}_x$  and  $\text{SO}_x$ , can be estimated. In this way it is possible to predict pollution concentrations such that they can be assessed and minimised by good design.

Radiation heat transfer in fires and flame tubes differs significantly in a number of ways. For the natural gas combustion processes considered in the present work, the thermal radiation field in a jet fire, for example, is highly anisotropic with significant levels of radiation in discrete spectral windows determined by the emitting species present in the combustion products and fuel. In an enclosed flame such as that present in a flame tube the radiation field is more isotropic and if significant levels of soot are present then the spectral radiation has a more continuous distribution in wave number space.

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