# Radiative heat transfer calculation in combustion systems

## Cálculo de transferêcia de calor por radiação em sistemas de combustão

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## Abstract

With an increasing trend towards cleaner combustion, accurate prediction of radiation of molecular gases is beginning to occupy a position of central importance in the design of gases-fired combustion appliances. The radiative heat transfer in absorbing- emitting gas mixtures can be most accurately predicted using line-by-line approach, but line-by-line calculations require large computer resources and computational time. Due to the increasing interest in applying the spectral integration of radiative transport equation in practical applications, several real gas models were developed. In the present work, a local-spectrum correlated model called cumulative wavenumber model (CW) is adopted and the spectral properties of the gases are obtained from HITRAN and HITEMP databases. The spectral radiative transport equation is solved using the CW model and the discrete ordinates method. Validation in gray and non-gray cases is presented by comparison with result of literature. Then, 2D axis symmetric furnace domain containing high temperature gases of combustion is modeled. The results are compared with a benchmark line-by-line results and Full Spectrum Correlated-k distribution model (FSCK) results taken of the literature. Scenarios investigated for non-isothermal and non-homogeneous mixtures of gases show that the CW approach is accurate to line-by-line solution. The development algorithms can be used in thermographic participating media calculations in combustion systems.

## Keywords

Radiation, Numerical Modeling, Real Gases, Non-isothermal, Cumulative Wavenumber.

## Introduction

Radiative heat transfer is the dominant mode of heat transfer in most combustion and fire applications and can significantly affect gas and wall temperatures. The treatment of radiative transport through combustion gases is rendered extremely difficult by the strong spectral variation of the absorption coefficients. Typical absorption spectra of gases such as $CO_2$, $H_2O$ and CO contain roughly $10^5$ to $10^6$ lines, and at combustion temperatures, higher than 2000 K, the number of lines present are well over a $10^6$ (EDWARDS, 1976); (ROTHMAN et al, 1992). From a modeling perspective, this implies that to accurately predict radiative transport in flames, one would have to solve the radiative transfer equation (RTE) for a million or so spectral intervals. Such computations are referred to as line-by-line (LBL) calculations, and require extraordinary large amounts of computer memory and time. For the vast majority high temperature systems, the most significant absorbing/emitting gaseous species are H2O, CO2, and CO.

In recent years, much attention has been focused on the solution of radiative transfer problems in high temperature gaseous media (TAINE and SOUFIANI, 1999) and due to the increasing interest in applying the spectral integration of radiative transport equation in practical applications, several real gas models were developed (DENISON; WEBB, 1993); (MODEST; ZHANG, 2002); (SOLOVJOV; WEBB, 2002).

Most practical combustion applications exhibit a variety of length scales with some regions of the domain containing much higher gradients than others. In many engineering applications, the solution of radiative transfer equation in the entire cavity for large systems is complicated and time consuming, but sometimes the interesting zone is only some local small domain. Due to the volume effect of radiative transfer, radiative transfer equation needs to be solved in the entire close cavity filled with participating me

dia. One spatial scheme that permits one adaptative and non-uniform grid is necessary in these cases, as the multidimensional scheme in (ISMAIL; SALINAS, 2004).

In the present work, the CW model (SOLOVJOV and WEBB, 2002) is adopted. This model needs the cumulative wavenumber function of distribution to treat the spectral variation of the absorption coefficients of the absorbing gases. The methods to construct and use this distribution function are outlined in (SOLOVJOV and WEBB, 2002; ISMAIL and SALINAS, 2005). In this work, the spectral properties of the gases are obtained from Hitran and Hitemp databases (ROTHMAN et al. 1998).

As an objective of the present work is the development and application of a general method to the spectral solution of the radiation heat transfer equations in mixtures of non-gray gases, in rectangular cavity and apply the results to model combustion systems with high temperature combustion gases, also it is expected for future works to use the development algorithms in thermographic application in combustion systems.


## Resumo

Devido ao aumento de pressões na busca de combustão limpa, a predição precisa da radiação de gases moleculares está começando a ocupar uma posição central no projeto de sistemas de combustão. A transferência de calor por radiação em misturas de gases absorventes e emissores de radiação pode ser estimada com grande aproximação utilizando o método Linha-por-Linha, mas os cálculos Linha-por-Linha requerem grandes recursos de computadores e grande tempo computacional. Devido ao aumento do interesse em aplicações práticas à integração espectral da equação de transporte radiativo, foram desenvolvidos vários modelos de gás real. Neste trabalho adotamos o modelo de correlação espectral local denominado modelo "Cumulative Wavenumber" (CW) e as propriedades espectrais dos gases são obtidas utilizando as bases de dados HITRAN e HITEMP. A equação espectral de transporte radiativo é resolvida utilizando o modelo CW e o método de ordenadas discretas. A validação em casos cinzentos e não cinzentos é apresentada em comparação com resultados da literatura. Então, é feita a modelagem de um forno simétrico em 2D contendo gases de combustão a alta temperatura. Os resultados são comparados com uma solução utilizando o método Linha-por-Linha e resultados do modelo FSCK tomados da literatura. Os cenários investigados para misturas de gases não isotérmicos e não homogêneos mostram que o modelo CW fornece resultados com similar precisão à solução Linha-por-Linha. Os algoritmos desenvolvidos podem ser utilizados em cálculos termográficos em meios participantes em sistemas de combustão.



## Palavras chave

Radiação, Modelagem Numérica, Gases Reais, Não Isotérmico, Modelo "Cumulative wavenumber".


## Formulation

### The radiative transport equation (RTE) in gray media

The radiative transport equation for an absorbing, emitting gray gas medium with isotropic scattering can be written as (SIEGEL and HOWELL, 1992),

$$(\Omega.\nabla)I(r,\Omega) = -(\kappa+\sigma)I(r,\Omega) + \frac{\sigma}{4\pi}\int_{4\pi} I(r,\Omega')d\Omega' + \kappa I_b(r) \qquad (1)$$

where $I(r,\Omega)$ is the radiation intensity in r, and in the direction ; , is the radiation intensity of the blackbody in the position r and at the temperature of the medium; is the gray medium absorption coefficient; is the gray medium scatter coefficient; and the integration is in incident direction $\Omega'$ . For diffusely reflecting surfaces the radiative boundary condition for Eq. (1) is

$$I(r,\Omega) = \varepsilon I_b(r) + \frac{\rho}{\pi}\int_{n.\Omega'<0} |n.\Omega'|\, I(r,\Omega')d\Omega' \qquad (2)$$

where r lies on the boundary surface , and Eq. (2)

is valid for n. >0. $I(r,\Omega)$ is the radiation intensity leaving the surface at the boundary condition, is the surface emissivity, is the surface reflectivity and n is the unit vector normal to the boundary surface.

The local divergence of the radiative flux is related to the local intensities by

$$\nabla.q_r = \kappa[4\pi \mathbf{I}_b(\mathbf{r}) - \int_{\Omega=4\pi} \mathbf{I}(\mathbf{r},\Omega')\mathbf{d}\Omega'] \qquad (3)$$

### The RTE in the cumulative wavenumber model

The radiative transport in an absorbing and emitting medium along a trajectory *S* in the direction W in spectral form is given by (SIEGEL and HOWELL, 1992),

$$\frac{\partial I_\eta}{\partial s} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta} \qquad (4)$$

As it is shown in Fig. 1, in the CW model (SOLOVJOV and WEBB, 2002), the total range of the absorption cross-section Ch is subdivided into supplementary absorption cross-section of gray gases $C_j$, $j$ = 1, ..., $n$, where $n$ is the number of gray gases. The intersection of the two spectral subdivisions is used to define the modeling of the fractional gray gas $D_{ij}$ and the sum of the fractional gray gases establishes the complete range of number of wave.

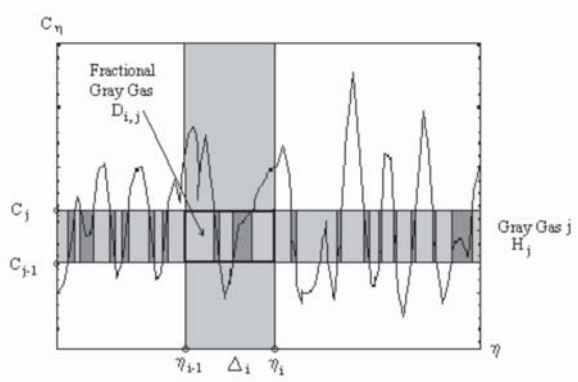

Figure 1 - CW modeling by fractional gray gases

In CW model (SOLOVJOV and WEBB, 2002), Eq. (4) is written as,

$$\frac{\partial J_{i,j}}{\partial s} = -\kappa_j J_{i,j} + \kappa_j J_{bi,j} \qquad (5)$$

where $J_{i,j}$ is the intensity of the fractional gray gas $D_{i,j}$ and $k_j$ is the absorption coefficient of gray gas determined by the equation,

$$\kappa_j = N_c \sqrt{C_j C_{j-1}} \qquad (6)$$

where $N_c$ is the molar density of the gas (molecules/cm$^3$).

The term $J_{bi,j}$ in Eq. (5) is the source radiative term at the black body fractional intensity

$$J_{bi,j}(s) = \int_{\Delta i} I_{b\eta}(T(s),\eta)\,d[\upsilon_{ij}(s)] = \int_{\Delta i} I_{b\eta}(T(s),\eta)\,d[W(C_j, s^*, \eta) - W(C_{j-1}, s^*, \eta)] \qquad (7)$$

where $W(C_j, s, h)$ is the cumulative wavenumber function as defined by Solovjov and Webb (2002) and $s^*$ is one spatial reference point where gas properties are known. The term $I_b$ $(T(s), h)$ is the black body spectral intensity. The Planck function is determined as the sum of the $J_{bi,j}(s)$ for all the fractional gray gases.

The boundary condition for non-gray walls, diffusively emitting and reflecting is,

$$I_\eta(s_w, \hat{\Omega}) = \varepsilon_{\eta w} I_{b\eta}(T_w) + \frac{\rho_{\eta w}}{\pi} \int_{n.\hat{\Omega}'<0} I_\eta(s_w, \hat{\Omega}')\,|n.\hat{\Omega}'|\,d\hat{\Omega}' \qquad (8)$$

where $s_w$ define the point on the frontier surface and the subscript $w$ refers to the quantity evaluated at the frontiers. $eh_w$ is the spectral emissivity and $rh_w$ is the spectral reflectivity of the frontier. Integration of Eq. (8) yields

$$J_{i,j}(s_w, \hat{\Omega}) = \varepsilon_{iw} J_{bi,j}(T_w) + \frac{\rho_{iw}}{\pi} \int_{n.\hat{\Omega}'<0} J_{i,j}(s_w, \hat{\Omega}')\,|n.\hat{\Omega}'|\,d\hat{\Omega}' \qquad (9)$$

When the equation of radiative transport, Eq. (5) together with the boundary conditions Eq. (9) are solved for all the fractional gray gases $J_{i,j}$, the total radiation intensity is determined from the sum of all intensities of gases with the correction factor $u_{i,j}(s)$ as weight (SOLOVJOV; WEBB, 2002).

$$I(s) = \int_0^\infty I_\eta(s)\,d\eta = \sum_{i,j} u_{i,j}(s) J_{i,j}(s) \qquad (10)$$

For any arbitrary point s, the function $u_{i,j}(s)$ can be calculated by the equation

$$u_{i,j}(s) = \frac{W(C_j, s, \eta) - W(C_{j-1}, s, \eta)}{W(C_j, s^*, \eta) - W(C_{j-1}, s^*, \eta)} \qquad (11)$$

For the case of isothermal and homogeneous media, Eq. (11) is reduced to $u_{i,j}(s) = u_{i,j} = 1$.



For a mixture of (g) gases of molar density $N_c$, the function $u_{i,j}(s)$ is defined according to Solovjov and Webb (2002), as

$$u_{i,j}(s) = \frac{\sum_g \left[W_g(C_j / Y_g) - W_g(C_{j-1} / Y_g)\right]}{\sum_g \left[W_g(C_j / Y_g) - W_g(C_{j-1} / Y_g)\right]} \qquad (12)$$

where $Y_g$ is the molar fraction of gas species.

The radiative source term for the gray gas $j$ is determined from equation

$$\nabla . q_{r,j} = 4\pi\kappa_j \sum_i J_{bi,j} - \sum_{m=1}^{M} w_m \kappa_j I_m \qquad (13)$$

and the total source term is written as

$$\nabla.q_r = \sum_j \nabla.q_{r,j} \qquad (14)$$

To discretize the spectral radiative transport equation in 2D using the CW model in every fractional gray gas *(i,j)*, one can rewrite Eq. (5) based upon the method outlined by Ismail and Salinas (2004), as,

$$(J^m_{i,j})^{n+1} = \frac{V_{i,j}(\kappa J_{bi,j})^n + |\mu_m| A_x (J^m_{i-\frac{1}{2},j})^{n+1} + |\xi_m| A_y (J^m_{i,j-\frac{1}{2}})^{n+1} + S^n_{df}}{|\mu_m| A_x + |\xi_m| A_y + \kappa V_{i,j}} \qquad (15)$$

where,

$$S^n_{df} = |\mu_m| A_x (I^m_{i,j} - I^m_{i+\frac{1}{2},j})^n + |\xi_m| A_y (I^m_{i,j} - I^m_{i,j+\frac{1}{2}})^n \qquad (16)$$

$S^n_{df}$ is the deferred correction term in nth iteration. Here, the spectral domain subscripts (i,j) are omitted and the space domain subscripts are (i,j), m indicate the mth direction of the angular quadrature, A is the area and V the volume of control volume (i,j).

The values of the fluxes in the faces a $(J^m_{i+\frac{1}{2},j})^n$ and $(J^m_{i,j+\frac{1}{2}})^n$ are interpolated using the CLAM or the genuinely multidimensional (GM) scheme (ISMAIL and SALINAS, 2004), while the values of the fluxes $(J^m_{i-\frac{1}{2},j})^{n+1}$ and $(J^m_{i,j-\frac{1}{2}})^{n+1}$ are interpolated using a step scheme. Several numerical experiments were realized to ensure that the algorithm does not have any directional march error and also to determine an adequate value for the over-relaxation factor.

## VALIDATION

The CW real gas model and the numerical algorithm are validated by comparison with the results of the

one 1D test case presented in Solovjov and Webb (2002), where the medium in this case is a homogeneous isothermal mixture of combustion gases at 1000 K and 1 atm total pressure occupying a gap of 5.0 m width between two parallel plates. The molar fractions of $H_2O$, $CO_2$ and CO in the mixture are 0.2, 0.1 and 0.03 respectively and the rest is nitrogen. The comparative results are shown in Fig. 2, and well accuracy is observed.

One second test problem is the solution of the radiative transport equation for a mixture of homogeneous isothermal gases in a two dimensional cavity. The gas media is a mixture of three gases of combustion. The mixture is homogeneous and isothermal at 1000 K and 1 atm total pressure occupying a two-dimensional square cavity of 1 m side. The molar fractions of $H_2O$, $CO_2$ and CO are 0.2, 0.1 and 0.03 respectively. The frontiers are black and non-emitting. The problem is solved using the spectral database HITEMP (ROTHMAN et al, 1998), at 1000K. Some numerical simulations were realized to investigate the convergence of the solution. The influence of refining the angular quadrature on the convergence of the solution is tested and it is found that for $T_n$ 6 and higher, the solution does not change and then indicating that the quadrature $T_n$ 6 is more adequate. Similarly, the effect of the size of the computational grid is evaluated and as a result of the numerical tests, the investigation is realized using the angular quadrature $T_n$ 6 with a grid of 20 x 20. By brevity these graphics are not shown here, see Ismail and Salinas (2005). Also, the algorithm is tested in reflecting boundaries and Fig. 3 shows the heat flux at walls of the cavity for the case of reflecting boundaries and is compared with result obtained in black boundary case. Consistent results are found.

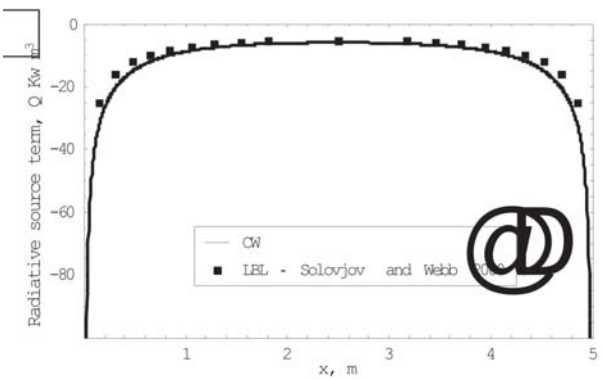


Figure 2 - Radiative dissipation source in gas mixture – 1D, Line-by-line solution of Solovjov and Webb (2002), CW model validation.

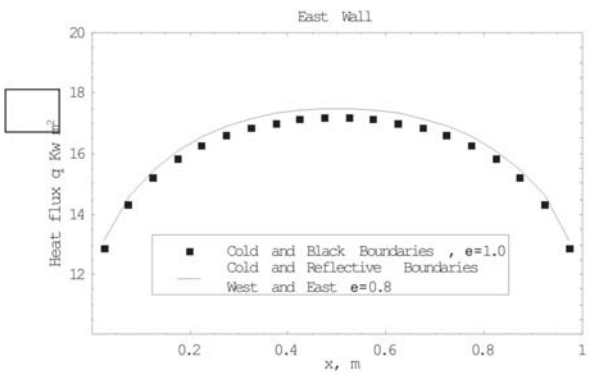


Figure 3 - Heat flux at east surface in two-dimensional cavity with an isothermal gas mixture at 1000 K, for north and south cold black walls and east and west cold reflecting walls.

## Radiative Modeling in Combustion Systems

The CW model is applied in a two-dimensional axisymmetric combustion system with non-isothermal gases. Two problems presented by Mazumder and Modest (2002), were solved. In the first one, the participant gas is $CO_2$. The geometry, boundary conditions, and operating parameters are shown in Fig. 4. The gas is non-isothermal and at 1 atm of total pressure. The molar fraction of $CO_2$ is 0.1 and the other gas present is $N_2$ (assumed non-participant) with 0.9 of molar fraction. The emissivity at all walls is 0.5, and gray isotropic scattering was considered, with scattering coefficient de 1 $m^{-1}$. The domain has three zones, two at 500 K and one intermediate zone at 2000 K. The reference temperature in the present simulation is selected equal to the colder temperature, 500 K. No changes in the solution were observed when the reference temperature was the higher temperature. The modeling is realized using 20 gray gases and a spectral interval $D_i$ = 100 $cm^{-1}$ with four spectral sub-interval $D_i$ = 25 $cm^{-1}$ in every one of them to accelerate the solution. The angular quadrature LC11 with 48 angular directions (KOCH and BECKER, 2004), and with a non-uniform grid of 12 x 12 is used. The results are plotted in the same scale presented in (MAZUMDER; MODEST, 2002), to facilitate the comparison with LBL and the Full Spectrum Correlated-k distribution (FSCK) results. The divergence of heat flux at three locations are shown in Fig. 5 and was compared with Line-by-Line solution taken of the Mazumder and Modest work (2002). It is observed that the CW results agree well with the LBL solution. It is also observed that CW model gives qualitatively similar approximation as FSCK model for the best strategy for temperature reference reported in (MAZUMDER; MODEST, 2002).

In the second problem, the participant gas is a mixture of combustion gases $CO_2$ and $H_2O$. The geometry, boundary conditions, and operating parameters are the same as shown in Fig. 4. The temperature and molar fractions in each zone are: Zone 1, 500 K, 0.05 $CO_2$, 0.1 $H_2O$; Zone 2, 2000 K, 0.1 $CO_2$, 0.2 $H_2O$; Zone 3, 500 K, 0.15 $CO_2$, 0.3 $H_2O$; and the other gas present is $N_2$ (assumed non-participant). The emissivity at all walls is 0.5, and gray isotropic scattering was considered, with scattering coefficient of 1 $m^{-1}$. The reference point in the present simulation is selected in the zone 1 and the reference values of temperature T(s*) and species concentration $Y_m$ (s*) are the corresponding values in the zone. No changes in solution were observed when the reference point was in other zone. The divergence of heat flux at three locations are shown in Fig. 6 and was compared with Line-by-Line solution taken from the Mazumder and Modest work (2002). It is observed that the CW results agree well with the LBL solution.

The CPU requirements for performing these calculations need to be mentioned at this point. The LBL calculations, involving about a million bands, requires about 2 days of CPU on an Intel Pentium III 733 MHz processor (MAZUMDER and MODEST, 2002). For the CW calculations, the total CPU required for five order of magnitude convergence involving 144 cells, 48 directions for LC11 DOM quadrature, two species and 20 gray gases and a spectral interval $D_i$ = 100 $cm^{-1}$ was about 40 min on a 866 MHz Intel Pentium III processor. In previous work (ISMAIL and SALINAS, 2005) the solution of the same problem but using 20 gray gases and a spectral interval $D_i$ = 25 $cm^{-1}$ was about 130 min on a 866 MHz Intel Pentium III processor. It was also necessary one day of CPU on a 866 MHz Intel Pentium III processor for convert spectral data from HITEMP database to CW model for each gas and temperature. Of course, the use of CW model requires generation de databases, but this is a one-time affair, and once a database is generated, it can be used for all cases. Similarly, Mazumder and Modest (2002) reported 20 days of CPU on a Pentium III 733 MHz processor for each gas with 18 reference temperatures for the FSCK model.

For all cases considered under this study, results were within 7% of LBL answers. Only at the position x equal 0.825 in the second case, the divergence with the LBL answers seems high, but in absolute value it was less to 0.02 of the dimensionless heat value.

## Conclusions

The local spectrum model and the cumulative wavenumber distribution function are applied to a mixture of real gases first in one-dimensional geometry to validate the numerical procedure and then extended to the two-dimensional cavity space with gray and reflecting boundaries in the isothermal cases. The model is tested in a strong non-isothermal and non-homogeneous cases and the results agree very well with LBL solutions. The selection of the reference point (temperature and species concentration reference) do not affect the solution. Also, the method and the algorithm can be used to solve the case with non-gray boundaries. To solve the radiative problem using the

CW model, the total CPU required for five order of magnitude convergence involving 144 cells, 48 directions for LC11 DOM quadrature, two species and 20 gray gases and a spectral interval $D_i$ = 100 $cm^{-1}$ was about 40 min on a 866 MHz Intel Pentium III processor. The method show ability to obtain faster solutions in participating media in combustion systems and can be applied in thermographic calculations in real gases thermal systems.

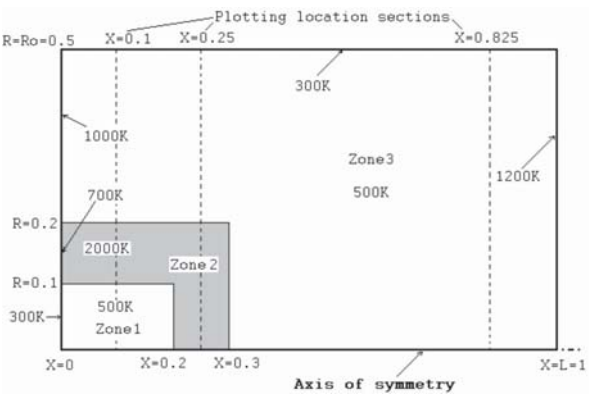


Figure 4 - Geometry, boundary conditions, and operating parameters for 2D non-isothermal case

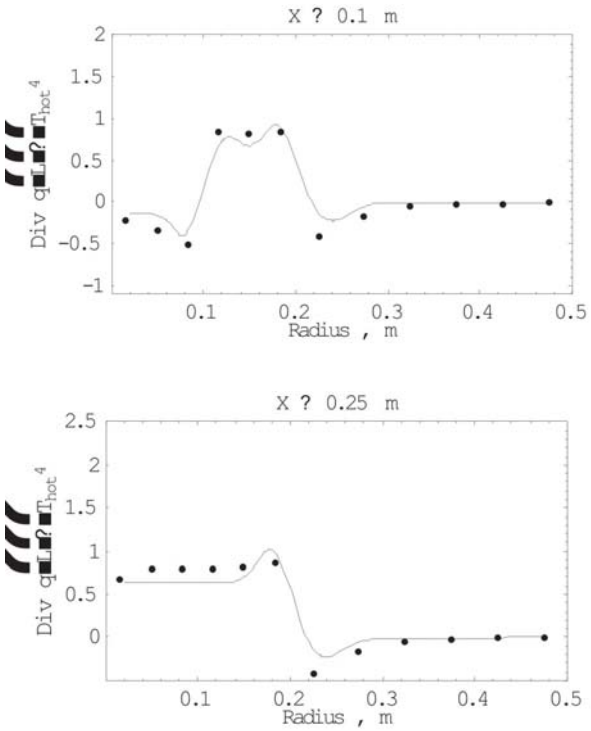


Figure 5 - Comparison of CW result with LBL results for non-isothermal gas case. CO2 at 0.1 molar fraction, (Line ¾¾ : solution LBL of Mazumder et al. (2002); Points · : CW solution)

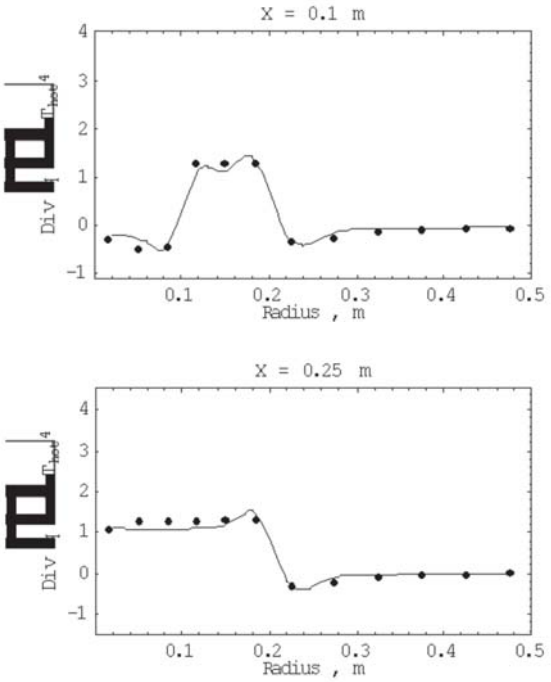


Figure 6 - Comparison of CW result with LBL results for non-isothermal gas mixture case.
(Line ¾¾ : solution LBL of Mazumder et al. (2002); Points · : CW solution)

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