Inverse Problem of Coupled Radiative and Conductive Heat Transfer in a Cavity Filled with CO2 and H2O at Different Mole Fractions

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ABSTRACT: This paper deals to an inverse analysis of combined conduction and radiation and heat transfer in a square cavity filled with radiating gases by numerical technique. The radiating medium is considered an air mixture with CO2 and H2O at different mole fractions, which is treated as homogeneous, absorbing, emitting and scattering gray gas. The main purpose is to verify the effects of gas mole fractions (carbon dioxide and water vapor) on the solution of inverse design problem. In the analysis, the conjugate gradient method is used to investigate the temperature distribution upon the heater surface to satisfy the prescribed temperature and heat flux distributions on the design surface. The temperature distributions over the heater surface while the enclosure is filled with different mole fractions of CO2 and H2O are calculated in this paper. It is found that the heater surface needs more power to maintain the design surface under uniform temperature and heat flux when the air mixture contains high mole fractions of CO2 and H2O. Numerical results reveal that by increasing the mole fractions of carbon dioxide and water vapor two times in the air mixture, the average heat flux over the heater surface increases about 16%. The present numerical results for the direct problems are compared with theoretical findings by other investigators and good consistencies are seen.

1- Introduction

Combined conduction and radiation heat transfer in a participating medium takes place in many engineering and industrial applications, such as in glass fabrication, furnaces, and combustion chambers, etc. These modes of heat transfer can be studied along direct or inverse problems. All boundary conditions in direct problems are known, while in inverse problems, some of the boundary conditions are unknown and must be calculated based on a desired condition along a boundary surface. In such cases, inverse boundary design analysis could be employed to achieve uniform temperatures or heat flux over some parts of a system [1]. One of the most well-known and powerful techniques to solve the integro-differential Radiative Transfer Equation (RTE) in a radiating medium is the Discrete Ordinates Method (DOM) [2]. Chandrasekar in 1950 [3] formulated this technique at first, and then DOM was modified by Carlson and Lathrop [4] in 60-70’s and Fiveland [5] and Truelove [6] in the 80’s.

Razzaque et al. [7] solved a conduction-radiation problem inside a two-dimensional rectangular geometry by numerical scheme. They used the finite element method to obtain the discretized forms of the governing equations. The product integration method was applied by Tan [8] to solve combined conduction-radiation problem in a square enclosure surrounded with isothermal walls. The discrete ordinate method was used for simulating the combined radiative and conductive heat transfer in rectangular enclosures by Kim and Baek [9]. For combined mode of heat transfer including conduction and radiation in two dimensional cavities, Rousse et al. [10] employed the Control-Volume Finite Element Method (CVFEM), and then the collapse dimension method by Talukdar et al. [11]. For simulating the coupled conduction and radiation heat transfer in two-dimensional planar geometry, Mahapatra et al. [12] employed a new hybrid method. Recently, the problem of combined conduction and radiation heat transfer in 2 Dimensional (2D) irregular geometries with anisotropic-scatter participating media was simulated numerically by Amiri et al. [13], using the DOM with the blocked-off technique.

All of the above mentioned studies are known as direct procedure which the whole boundary conditions and fluid properties of radiating media are determined as input data to distinguish the temperature of medium and wall heat flux distributions whereas in inverse method, boundary conditions or thermophysical properties could be unknown and must be determined. Inverse analysis can be used to calculate boundary conditions, heat source profile and so on. Optimization and regularization methods were applied by many investigators to recognize unknown intensity of heater surface in enclosures with combined conductive-radiative heat transfer [14-19]. Sarvari et al. [20] and Sarvari [21] studied inverse combined conduction and radiation boundary design problem in irregular 2D geometries. They used the conjugate gradient method to find the unknown heater power in order to satisfy pre-specified temperature and heat flux over design surface. Das et al. [22] used the genetic algorithm in a transient 2D conduction-radiation problem. They applied

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the Lattice-Boltzman method to solve the energy equation. Estimation of applied heat flux at the surface of ablating materials by using sequential function specification method was numerically solved by Farzan et al. [23]. Recently, an inverse forced convection–radiation boundary design problem for a two dimensional channel with a forward and a backward-facing step has been solved by Bahraini et al. [24]. Omidpanah and Gandjalikhani Nassab [25] solved an inverse analysis of combined radiation and convection heat transfer in a 2D rectangular duct. The working fluid is a mixture of air including CO$_2$ and H$_2$O as two radiating gases. It is revealed that increase in mole fraction of gases mixture leads to a heater surface with higher power input.

As a recent study in inverse problem, the inverse analysis of radiative flux maps for the characterization of high flux sources was done by Suter et al. [26]. In that study, the aim was the determination of intensity distributions of arbitrarily complicated concentrating facilities.

According to the literature survey and to the best of author’s knowledge, the inverse boundary design procedure has not been established in combined conduction-radiation heat transfer in square cavity filled with different types of radiating media. This problem can show how the solution of inverse design is affected by the type of radiating media which is a mixture of air with water vapor and carbon dioxide with different mole fractions. The selection of CO$_2$ and H$_2$O in the present work is due to this fact that these are two radiating gases with almost high absorption coefficient. The Planck mean absorption coefficient is calculated across spectrum $1500 \text{cm}^{-1}$ to $9000 \text{cm}^{-1}$ using the line-by-line calculations. The aim is to find the unspecified temperature distribution on the heater surface to satisfy both uniform temperature and heat flux distributions on the design surface for different values of gas mole fractions [27]. The fluid is considered to be a homogenous gray absorbing-emitting-scattering medium, and all physical properties are assumed to be uniform. The cavity walls are treated as gray-diffuse absorbers and emitters. An optimization technique according to the conjugate gradient method is used for minimizing an objective function. The finite difference method is used to solve energy equation and the radiative transfer equation is solved with DOM [1].

It should be noted that the effect of gas properties variation by changing mole fraction on the solution of inverse conductive-radiative problem has been done for the first time in present work. All computations and numerical simulations are coded into a FORTRAN computer code by the authors.

2- Problem Description

A schematic view of the two dimensional square cavity with length L, which is filled with a homogenous mixture of air with two radiating gases is shown in Fig. 1. The heater surface with length L is located on the whole of the top wall, while the design surface is located on the middle of the bottom wall with length L/2. Side walls are kept at 400 K, while the design surface and bottom wall temperatures are equal to 380 K. The cavity walls have constant emissivity equal to 0.8. It is desired to determine the unspecified temperature profile on the heater surface for satisfying uniform temperature of 380 K and constant heat flux equal to $-200 \text{ W/m}^2$ over the design surface.

3- Theory

The energy equation for combined radiation and conduction heat transfer in a participating medium at the Cartesian coordinate system under steady state condition with constant properties is as in Siegel and Howell [28]:

$$k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - \nabla q_r = 0$$

(1)

To solve Eq. (1), the divergence of the radiative heat flux $\nabla q_r$ is related to the temperature distribution inside the medium as below [1]:

$$\nabla q_r = k \left( 4 \pi I_s (r) - G(r) \right)$$

(2)

In Eq. (2), $G(r)$ is incident radiation defined as:

$$G(r) = \int \frac{I(r, \Omega) d\Omega}{4 \pi}$$

(3)

To calculate both radiation intensity field and $\nabla q_r$, it is essential for solving of the radiative transport equation. This equation for an emitting, scattering and absorbing gray medium is in Modest [29]:

$$\left( \Omega, \nabla \right) I(r, \Omega) = -\beta I(r, \Omega) + \kappa I_s (r) + \frac{\sigma_t}{4\pi} \int I(r, \Omega') \phi(\Omega, \Omega') d\Omega'$$

(4)

In which, $I_s (r)$ is the blackbody radiation intensity in the
The radiative boundary condition for Eq. (4) for a diffusely reflecting surface, is

\[ I(r, \Omega) = \epsilon I_b(r) + \frac{\rho}{\pi} \int_{\Omega_r} I(r, \Omega') n_{\Omega} d\Omega' \tag{5} \]

where, \(r\) denotes the boundary surface, \(I(r, \Omega)\) is the radiation intensity leaving the boundary surface, \(\epsilon\) is the emissivity of the surface, \(\rho\) the surface reflectivity, and \(n\) is the unit vector normal to the boundary surface. In the present study, the Planck mean absorption coefficient is used as an averaged absorption coefficient obtained from the line-by-line calculations as [29]:

\[ \kappa_p = \frac{\int_0^\infty I_b(\beta, \sigma) d\sigma}{\int_0^\infty I_b(\beta, \sigma) d\beta} \tag{6} \]

Such that the non-gray radiation gas is replaced by its equivalent gray one and the RTE is solved independent of wave number that needs less computations. In this study, the average temperature \(T_{avg}\) at which the Planck mean absorption coefficient is calculated is equal to 400 K. The absorption coefficient is computed across the spectrum \(\eta \sim 50 \text{cm}^{-1} < \eta < 20000 \text{cm}^{-1}\) based on the HITRAN 2008 database [30] using 457500 lines.

The following non-dimensional parameters are used to describe the results of the present work:

\[ (X, Y) = \left( \frac{x}{L}, \frac{y}{L} \right), \quad RC = \frac{T_{av}^3 L}{k}, \tag{7} \]

\[ Q = \frac{q}{\sigma T_{av}^3}, \quad \omega = \frac{\sigma_s}{\beta}, \quad \theta = \frac{T - T_d}{T_{ave} - T_d} \]

4- Inverse Problem

In the present inverse problem, the conjugate gradient method is applied to estimate the unknown temperature profile, \(T_h(x)\) on the heater surface. The conjugate gradient method works based on minimizing an objective function, \(G\), which is defined as follows [1, 31]:

\[ G = \sum_{n=1}^{N}(Q_{d,n} - Q_{e,n})^2 \tag{8} \]

The dependent variables \(Q_d\) and \(Q_e\) are the estimated and desired heat fluxes, respectively, \(N\) is the number of nodes and \(n\) the node number on design surface. According to the following relation, the heater surface temperature at iteration level \(k+1\) is updated based on its value at previous iteration level.

\[ T_{h,m}^{k+1} = T_{h,m}^k - \psi^k d_m^k \tag{9} \]

In Eq. (9), \(\psi^k\) is the search step size at \(k\) level of iteration procedure and \(d_m^k\) is direction of descent that can be computed as:

\[ d_m^k = \nabla G_m^k + \gamma^k d_m^{k-1} \tag{10} \]

In Eq. (10), \(\gamma\) is the conjugate coefficient which is stated as below [1]:

\[ \psi^k = \sum_{m=1}^{M} \left( \nabla G_m^k \right)^2 \]

For calculating the value of \(\nabla G\), Eq. (8) must be differentiated with respect to unknown parameter \(T_{h,m}\). Thus:

\[ \nabla G_m^k = -2 \sum_{n=1}^{N} J_{mn}^k (Q_{d,n} - Q_{e,n}) \tag{12} \]

In Eq. (12), \(J_{mn}^k = \frac{\partial Q_m^k}{\partial T_{h,m}^k}\) is the sensitivity coefficient. Accordingly, the search step size can be obtained as follows [27]:

\[ \psi^k = \frac{\sum_{m=1}^{M} \sum_{n=1}^{N} (J_{mn}^k)^2 (Q_{d,n}^k - Q_{e,n}^k)}{\sum_{m=1}^{M} \sum_{n=1}^{N} (J_{mn}^k)^2} \tag{13} \]

4- 1- Sensitivity problem

For calculation of the sensitivity coefficients, the governing equations and boundary conditions are differentiated with respect to heater temperature. The differentiated forms of the energy and radiative transfer equations are as follows [1]:
The computational procedure is summarized below. The detail of numerical method is summarized here. Calculation is started with an initial guess for the unknown temperature distribution inside the medium, \( T_0(X) \), set \( k = 0 \) and then the following steps are performed [1]:

Step 1. Temperature distribution inside the medium is obtained from step 1, the sensitivity problem is solved [1].

Step 4. The conjugation coefficient and the gradient direction are calculated by Eqs. (11) and (12).

Step 5. The direction of descent, \( \Delta_x \) and the search step size, \( \eta \), are obtained by Eqs. (10) and (13), respectively.

Step 6. The new estimation for \( T_{h, m}^d(a) \) is calculated, computations are continued by step 1.

Since calculation of sensitivity matrix is a time-consuming procedure when the number of elements to be computed is massive, operating with the optimized grid is essential to include grid-independent solutions and also to reduce the time of computations. Thus, along a direct problem which is a square cavity with isotherm walls, the distribution of total heat flux on the bottom wall are calculated at different grid sizes. It is seen in Fig. 2 that the optimized mesh size \( 40 \times 40 \) can be used for subsequent computations.

6- Validation

For validation, the present numerical method for a direct problem is applied to analyze the unit square cavity studied by Mahapatra et al. [12]. The enclosure contains radiating gas and has isotherm and black walls with specified boundary conditions as it is shown in Fig. 3 [1]. This figure also depicts the variation of mid-plane temperature distribution inside the cavity which is obtained by numerical solution of the RTE and energy equation. Comparison between the present results with those obtained by Mahapatra et al. [12] shows excellent agreement.

To verify the accuracy of inverse problem, we use the results of previous problem in mesh study for analyzing combined radiation conduction heat transfer in a square cavity [27].

After insuring verification of the direct problem, total heat flux distribution upon the bottom wall of the cavity as the design surface is considered as additional information for an inverse problem [1]. In inverse problem, the bottom and top walls of cavity are considered to be the design and heater surface, respectively. Now, the problem is to investigate the unspecified distribution of temperature over the heater surface placed on the top wall, to obtain both uniform temperature and specified heat flux distributions over the design surface. All boundary conditions and physical properties are the same.
as those applied in Fig. 2.

As we expect, the heater must be at uniform temperature all over its surface. Fig. 4 shows the calculated and the exact temperature variations over the heater surface. As it is seen, there is a good consistency between the predicted and exact temperature distributions where the maximum errors happen at two ends. It is due to this fact that the two ends, (X=0, 0.1) are two singular points located at the interfaces of side walls (T=400 K) with the top wall (T=420 K) where the temperature continuity along the cavity boundary surface vanishes. It is evident that this weakness introduces some errors more than the interior points as it is seen in Fig. 4.

7- Results

The 2D square cavity shown in Fig. 1 which is filled with a homogenous mixture of radiating gases is considered in the present work. All walls are diffuse-gray with constant emissivity equal to $\varepsilon_x = \varepsilon_y = \varepsilon_z = 0.8$. The side walls are kept at 400 K and the design surface and the bottom wall have a uniform temperature of 380 K. Besides, a uniform heat flux of $Q = -200 \text{ W/m}^2$ is imposed on the design surface.

The propose is to study the effect of gas mole fractions and some other different parameters such as radiation-conduction parameter and scattering coefficient on the power of heater as a heat source. As it was mentioned before, in reality the mixture of air with water vapor and carbon dioxide has non gray behavior and its absorption coefficient depends to the wave number as it is demonstrated in Fig. 5. But in the computations, the radiating gas is considered to be gray and the Planck mean absorption coefficient is employed in simulation.

First, to demonstrate the pattern of temperature distribution inside the cavity, the isotherms are drawn in Fig. 6. It is seen that the domains with high temperature gradients are near to the heater surface (as the energy source) and design surface (as the sink). This figure shows a special temperature distribution over the top wall to maintain the design surface at uniform temperature of 380 K. Since, the design surface is imposed with incoming heat flux of $-200 \text{ W/m}^2$, it should be located inside the low temperature region of the cavity as it is depicted in Fig. 6.

The effect of gas mole fractions on the temperature distribution along the heater surface in two cases of combined radiation conduction heat transfer and pure radiation is studied as the main goal of this paper. Fig. 7 shows the temperature distributions over the heater surface at different
mole fractions of the radiating gas components. As seen in Fig. 7, heater temperature is much affected by H$_2$O and CO$_2$ mole fractions, such that higher temperature over the heater surface is needed by increasing in gas mole fractions. Besides, the heater surface has different temperature patterns with different gas mole fractions. It should be noted that by increasing in the mole fraction of radiating gases in the mixture, the radiative absorption of the mixture increases and the participating medium becomes more radiative. If one compares the heater temperature distributions in the cases of radiation conduction and pure radiation heat transfer with each other, it can be found that with omitting the conduction heat transfer mechanism, high rate of heat transfer from the heater surface is needed to maintain the design surface at the desired uniform temperature and heat flux. Among the case studies in Fig. 7, the heater surface in the pure radiation case with 20% H$_2$O and 10% CO$_2$ needs the greatest temperature and therefore more input power.

In Fig. 8, the variations of total heat flux distribution on the heater surface are plotted. This figure is in consistent with the previous one, such that high rate of heat transfer takes place over the heater surface by increasing in the amount of gas mole fractions, especially in the case of pure radiation.

The distributions of relative error ($E_{rel}$) of the estimated heat flux over the design surface at different values of the gas mole fractions are presented in Fig. 9. The relative error is defined as:

$$E_{rel} = \frac{|Q_{d,n} - Q_{e,n}|}{Q_{d,n}} \times 100$$

Fig. 9 shows that the relative error has different trends over the design surface in the cases of having different gas mole fractions. Such that the relative error is approximately large near the two edges of the design surface in comparison to other parts for 20% H$_2$O and 10% CO$_2$, but when these mole fractions decrease to their half values, minimum values of the relative error occur at the two edges. However, it should be mentioned that in all cases, the value of relative error is less than 0.3%.

One of the main parameters in the design of high temperature thermal systems is the Radiation-Conduction (RC) parameter which indicates the significance of the radiation heat transfer relative to conduction counterpart. High values of RC parameter shows that radiation is the dominant mode of heat transfer in thermal system. In order to investigate the effect of RC parameter in the inverse design problem, the temperature distribution over the heater surface at three different values of RC are computed and drawn in Fig. 10. This figure also consists the case of pure radiation which coincides with infinite value of the radiation conduction parameter. As seen, high temperature for the heater surface is computed for large values of RC and the highest for the pure radiation case.

In order to have a better understanding of the thermal behavior of system, the total heat flux distributions over the heater surface at different values of the RC parameter are presented in Fig. 11. This figure shows different patterns
for the distribution of heat flux on the heater surface by changing RC parameter, such that in the case of $RC = 10$, the minimum value of heater heat flux takes place at the middle of it but for other cases, the maximum value of heat flux happens there. Also, Fig. 11 shows that by increasing in radiation conduction parameter, total heat flux over the heater surface increases which is in consistence with the founding by the previous figure. According to Fig.11, one can find that a designer prefers to have thermal systems with low values of the RC parameter in comparison to high values ones, since the heaters installed on the heater surface needs much less power. It is also seen that no parts of the heater surface have zero or negative heat flux (cooling on the heater surface!), so the solution achieved by the inverse method for this case is a realistic one.

8- Conclusion
The present work describes the inverse boundary design in a cavity filled with a mixture of radiating gases with different mole fractions. The temperature distribution on the heater surface was determined for having the specified temperature and heat flux distributions along the bottom wall of cavity as design surface. The theoretical formulation was explained by a set of high non-linear equations govern to a combined radiation-conduction heat transfer in a cavity. The DOM was used for calculation of radiant intensity from the radiative transfer equation, while the energy equation was numerically solved by the finite volume method. In the present inverse problem, the well known conjugate gradient method was used for calculation of the temperature of heater as a heat source. The relative error in the computation of heater temperature in all case studies was less than 0.3%. This makes the investigation more realistic. Numerical results showed that the gas mole fractions and conduction-radiation parameter have considerable effects on the result of such inverse problem. In this regard, numerical results reveal that by increasing the mole fractions of carbon dioxide and water vapor two times in the air mixture, the average heat flux over the heater surface increases about 16%.

Fig. 10. Temperature distribution over the heater surface at different values of the RC parameter

Fig. 11. Total heat flux distribution over the heater surface at different values of the RC parameter

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d$</td>
<td>Direction of descent</td>
</tr>
<tr>
<td>$E$</td>
<td>Error</td>
</tr>
<tr>
<td>$G$</td>
<td>Objective function</td>
</tr>
<tr>
<td>$H$</td>
<td>Height of the channel, m</td>
</tr>
<tr>
<td>$I$</td>
<td>Radiation intensity, W/m$^2$</td>
</tr>
<tr>
<td>$J$</td>
<td>Sensitivity matrix</td>
</tr>
<tr>
<td>$k$</td>
<td>Thermal conductivity, W/m.K</td>
</tr>
<tr>
<td>$M$</td>
<td>Number of nodes on heater surface</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of nodes on design surface</td>
</tr>
<tr>
<td>$q$</td>
<td>Heat flux, W/m$^2$</td>
</tr>
<tr>
<td>$Q$</td>
<td>Dimensionless heat flux</td>
</tr>
<tr>
<td>$RC$</td>
<td>Radiation-conduction parameter</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature, K</td>
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<tr>
<td>$w$</td>
<td>Quadrature weight associated with the direction,$s$</td>
</tr>
<tr>
<td>$x,y$</td>
<td>Dimensional coordinates, m</td>
</tr>
<tr>
<td>$X,Y$</td>
<td>Dimensionless coordinates</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Extinction coefficient, 1/m</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Dirac delta function</td>
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<tr>
<td>$\varepsilon$</td>
<td>Wall emissivity</td>
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<tr>
<td>$\phi$</td>
<td>Scattering phase function, inclination angle</td>
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<tr>
<td>$\gamma$</td>
<td>Conjugate coefficient</td>
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<td>$\eta$</td>
<td>Derivation of radiation intensity with respect</td>
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<td>Dimensionless temperature</td>
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<tr>
<td>$\sigma$</td>
<td>Stefan Boltsman’s constant</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Absorption coefficient, 1/m</td>
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<tr>
<td>$\sigma_s$</td>
<td>Scattering coefficient, 1/m</td>
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<tr>
<td>$\omega$</td>
<td>Scattering albedo</td>
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<tr>
<td>$\psi$</td>
<td>Search step size</td>
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<tr>
<td>$\zeta$</td>
<td>Derivation of temperature with respect to the heater element</td>
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<tr>
<td>$avg$</td>
<td>Average</td>
</tr>
<tr>
<td>$B$</td>
<td>Bottom</td>
</tr>
<tr>
<td>$d, D$</td>
<td>Design surface, desired heat flux</td>
</tr>
</tbody>
</table>
\[ h, H \quad \text{Heater surface} \]
\[ k \quad \text{Iteration number} \]
\[ L \quad \text{Left} \]
\[ m \quad \text{Node number on heater surface} \]
\[ n \quad \text{Node number on design surface} \]
\[ r, R \quad \text{Radiation, right} \]
\[ \text{rel} \quad \text{Relative} \]
\[ w \quad \text{Wall} \]
\[ R \quad \text{Radiative} \]
\[ T \quad \text{Total} \]

References


