Research Paper

Inverse identification of boundary conditions in a scramjet combustor with a regenerative cooling system

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HIGHLIGHTS

- Boundary condition of scramjet combustor is inversely identified for first time.
- The FEM in the ABAQUS software is employed to solve the direct problem.
- The identification is accurate, efficient, stable and robust.
- The identification methodology is promising in further practical applications.

ABSTRACT

Accurately determining boundary conditions in a scramjet combustor is of great importance for modeling the coupled process of fuel burning, fluid flow and heat transfer in the scramjet combustor, and for design and optimization of the cooling system. In this paper, a new methodology is proposed for determining boundary conditions at inaccessible surfaces of a scramjet combustor with a regenerative cooling system, which are identified by solving a three-dimensional transient inverse heat conduction problem. The finite element method in the ABAQUS is employed to solve the direct heat conduction problem in the scramjet combustor with the regenerative cooling system. A gradient-based method is used to solve the inverse problem attributed to its high accuracy and efficiency, and temperatures at accessible positions provide additional information for the inverse analysis. Examples are given to examine the performances for identifying boundary conditions in a scramjet combustor with a regenerative cooling system.

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1. Introduction

Scramjets are commonly employed in hypersonic vehicles, in which the temperature could reach more than 3000 K \cite{1}, and the thermal protection system \cite{2} is of great importance for the safety of scramjets. Passive thermal protection technique \cite{2} could not meet the demand of the flight time varying from minutes to hours of hypersonic vehicles. Therefore, an active thermal protection technique is necessary and the regenerative cooling technique \cite{3} is generally regarded as the most prospective. For the regenerative cooling system of a scramjet, accurately determining the boundary conditions in the scramjet combustor is a key issue for design and optimization of the cooling system, which has been studied in some papers \cite{4-6}. However, it is usually difficult involving complex fuel burning, fluid flow and heat transfer modeling \cite{7-14}, or not very reliable due to empirical formula, or partly carried out in experiments, which are disadvantageous for design and optimization of the cooling system for a scramjet combustor.

In the present work, a new methodology is proposed to determine the boundary conditions in a scramjet combustor. Boundary conditions at inaccessible surfaces of a scramjet combustor will be identified by solving a three-dimensional transient inverse heat conduction problem, by utilizing temperatures at measurable/accessible positions. While determination of boundary conditions by solving an inverse heat conduction problem has been reported \cite{15}, it is the first time to inversely estimate boundary conditions for a scramjet combustor with the regenerative cooling system to the best of the authors’ knowledge. Moreover, the present work has great application values for both design and optimization of the regenerative cooling system.

To inversely identify boundary conditions in a scramjet combustor, solutions to both direct and inverse problems are important. To solve direct heat conduction problems, the finite difference method (FDM) \cite{16}, the finite element method (FEM) \cite{17}, the boundary element

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1359-4311/ © 2018 Elsevier Ltd. All rights reserved.
method (BEM) [18], the meshless method (MLM) [19], and the finite volume method (FVM) [20] are frequently used. Each method has both advantages and disadvantages, and the FEM is the most suitable to solve multidimensional heat conduction problems in complex structures or in engineering applications and there are some available commercial software, such as ANSYS, ABAQUS, NASTRAN and so on. Therefore, the three-dimensional transient heat conduction problem is to be solved by using the FEM in the ABAQUS in the present work. To solve inverse heat transfer problems, a lot of methods were innovatively proposed, such as the conjugate gradient method [21–25], the Levenberg–Marquardt method [26–28], the krill herd algorithm [29], the Fourier transform [30], the genetic algorithm [31,32] and fundamental solutions [33], the Kalman filter method [34,35], a domain decomposition Method [36], the particle swarm optimization algorithm [37], and the singular value decomposition [38], which were partly reviewed in Refs. [39,40]. These methods could be divided into two groups: the stochastic and the gradient ones [40]. The former could search a global optimal solution, but they may require many iteration numbers. While the latter are more suitable to be adopted if one could estimate the range of the inverted parameters, attributed to sufficient accuracy and efficiency [41–47]; boundary conditions or thermo-physical properties have been estimated. In the present work, a gradient method, i.e., the Least-squares method [41], will be employed to solve the inverse heat conduction problem.

In the present work, two challenges are encountered by using the FEM in the ABAQUS and the Least-squares method for identifying boundary conditions in a scramjet combustor with the regenerative cooling system. First, the complex-variable-differentiation method (CVDM) [48], which has been employed for accurately calculating sensitivity coefficients in the previous work [40–42], cannot be used in the present work, because the complex-variable-differentiation method is unavailable in the ABAQUS. Second, data exchange has to be automatically carried out between intermediate results and input/output files of the ABAQUS. Some specific data in the input file have to be automatically revised, and some results have to be automatically extracted from the strings in the output file of the ABAQUS. To solve the first problem, an alternative method is adopted to calculate sensitivity coefficients without the CVDM. To deal with the second issue, program codes are also introduced. The new methodology is validated by using

The remainder of this paper is as follows. In Section 2, the three-dimensional transient heat conduction problem is described. Section 3 briefly reviews the Least-squares method, in which additional program codes are also introduced. The new methodology is validated by using
experimental data in Section 4. In Section 5, the efficiency, accuracy coupled with effects of initial guesses and measurement errors for identifying boundary conditions in a scramjet combustor with the regenerative cooling system are investigated. Conclusions are drawn in Section 6.

2. Direct problem: three-dimensional transient heat conduction problem

The three-dimensional transient heat conduction problem can be described using the following energy equation:

$$\rho C \frac{\partial T(x,y,z)}{\partial t} = \lambda \left[ \frac{\partial^2 T(x,y,z)}{\partial x^2} + \frac{\partial^2 T(x,y,z)}{\partial y^2} + \frac{\partial^2 T(x,y,z)}{\partial z^2} \right]$$  \hspace{1cm} (1)

with the initial condition

$$T(x,y,z,0) = T(x,y,z)$$  \hspace{1cm} (2)

and boundary conditions

$$-\lambda(T) \frac{\partial T(x,y,z,t)}{\partial n} = q_i(x,y,z,t)$$  \hspace{1cm} (3)

$$q(x,y,z,t)|_{\partial S} = h(T_i-T_f)$$  \hspace{1cm} (4)

The direct problem is to calculate the temperature field for the inverse analysis. In the present work, the FEM in the ABAQUS is employed to solve the three-dimensional transient heat conduction problem in the complex structure.

3. Inverse problem

In the inverse problem, boundary conditions on some surfaces of the scramjet combustor with the regenerative cooling system are unknown and need to be identified, but everything else in the direct problem is known. Temperature measurements at some accessible positions are necessary for the identification of the boundary conditions. The objective function for identifying boundary conditions is as follows.

$$S(q_1,q_2,\ldots,q_M) = \frac{1}{M} \sum_{i=1}^{M} \left( \frac{T_i - T_i^*}{T_i^*} \right)^2$$  \hspace{1cm} (5)

The inverted parameters vector can be updated by:

$$\delta q_{k+1}^* = \delta q_k^* + \delta^t$$  \hspace{1cm} (6)

where $\delta$ is determined from

$$J^T[J] \delta = J^T[T_i^* - T_i(q)]$$  \hspace{1cm} (7)

The sensitivity coefficients matrix in Eq. (7) can be determined from:

$$J = \begin{bmatrix} \frac{\partial T_i}{\partial q_1} & \frac{\partial T_i}{\partial q_2} & \cdots & \frac{\partial T_i}{\partial q_M} \\ \frac{\partial T_2}{\partial q_1} & \frac{\partial T_2}{\partial q_2} & \cdots & \frac{\partial T_2}{\partial q_M} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial T_M}{\partial q_1} & \frac{\partial T_M}{\partial q_2} & \cdots & \frac{\partial T_M}{\partial q_M} \end{bmatrix}$$  \hspace{1cm} (8)

It can be seen from Eqs. (4)–(8) that determining each sensitivity coefficient in $J$ matrix is a key step. The complex-variable-differentiation method (CVDM) [48] was employed to accurately calculate each sensitivity coefficient in our previous work. However, the CVDM is ineffective and could not be adopted in the present work, because the CVDM is based on our in-house program codes, and no source codes are available in the ABAQUS. Therefore, an alternative method, i.e., the central format of a finite difference method [49] is used for sensitivity analysis in this paper.

The iteration is stopped until the objective function or the difference between $S^{k+1}$ and $S^k$ is within a specified tolerance.

$$S^k < \xi$$ or $|S^{k+1}-S^k| < \xi$  \hspace{1cm} (9)

In this paper, one of main tasks is to develop additional program codes to automatically call the FEM in the ABAQUS, and automatically exchange data between intermediate results and the input/output files of the ABAQUS. This is because the direct problem has to be automatically solved in each iterative process, not just operating the friendly interface as usual. Moreover, the required iteration number is generally more than one. The data exchange process has to be automatically carried out by using program codes, for each iteration, between intermediate results and the input/output files of the ABAQUS.
Therefore, additional FORTRAN program codes have been developed to realize the above-mentioned functions. Boundary conditions at specific surfaces in the input file for the ABAQUS are automatically revised at each iteration by using the initial guessed or resulted values in the Least-squares method. Temperatures at measurement points are automatically extracted from strings in the output file of the ABAQUS. The solution procedure for identifying boundary conditions in a scramjet combustor with the regenerative cooling system can be summarized as follows.

Step 1. Solve the three-dimensional transient heat conduction problem based on \( q_0 \) for boundary conditions.

Step 2. Extract the temperature values at measurement positions from the output file of the ABAQUS.

Step 3. Check the stopping criterion. Stop the iteration if the stopping criterion is achieved. Otherwise, continue the following procedure.

Step 4. Calculate each value of \( \frac{\partial T}{\partial q} \) by using the finite difference method, and solve Eq. (7) to obtain \( \delta \).

Step 5. Update \( q_0 \) by Eq. (6), and write the values into the input file for the ABAQUS. Then return to Step 1.

The flowchart is shown in Fig. 1.

4. Validation of the present methodology

The present methodology is first validated before its application in inversely identifying boundary conditions in a scramjet combustor with a regenerative cooling system. The experimental data in Ref. [15] is employed. The direct heat conduction problem is one-dimensional, and the transient experimental temperatures at the 1/4, 1/2 and 3/4 depth are shown in Fig. 2. Thermo-physical properties, geometrical conditions, as well as initial conditions are known, which have been given in Ref. [15]. Boundary heat flux on the upper and bottom surfaces are inversely identified by using the present methodology and utilizing the experimental data in Fig. 2. Fig. 3 shows identified results by using the present methodology and those in Ref. [15]. It can be seen that they agreed very well, which validates the high accuracy of the present methodology.

5. Examples for identifying boundary conditions in a scramjet combustor

Fig. 4 shows one of outer wall structures of a scramjet combustor with regenerative cooling channels designed inside the wall structures. There are 14 regenerative cooling channels for the entire scramjet combustor in the present work, and only one channel is selected which is shown in Fig. 5, considering that the heat transfer mechanism is nearly the same in each channel. To identify boundary conditions in a scramjet combustor with the regenerative cooling system, the cooling channel must be taken into account in the selected structure with appropriate FEM model. The selected structure is 0.2 m in length, 0.005 m in width, and 0.019 m in height; the selected channel whose diameter is 0.0015 m is located inside it. The domain is the entire solid structure in Fig. 5, and it should be emphasized that the channel is hollow.

In the direct problem, the initial temperature is 1400 K, and the time is 200 s. The conductivity is 14.7 W/(m·K). The density and specific heat are 8240 kg/m³ and 481.4 J/(kg·K), respectively. The heat flux on the boundary of the scramjet combustor (bottom surface in Fig. 5) is distributed with positions, and the values at three representative positions are 460 kW/m², 480 kW/m², and 500 kW/m², respectively. The inner surface of the cooling channel is imposed on convective boundary condition (B. C.), and the convective heat transfer coefficient and the temperature of the fuel/coolant are 500 W/(m²·K) and 300 K.
respectively. All the other boundaries are adiabatic. The boundary conditions are illustrated in Fig. 5. Fig. 6 shows the FEM model for the ABAQUS, in which unstructured grids are adopted, and there are 23,188 nodes and 109,992 elements, respectively. Fig. 7 shows the transient temperature field by using the FEM in the ABAQUS for solving the direct problem. It can be seen that the transient temperature field increases with the time, and the heat gradually conducts from the combustor surface to other positions. This is because the heat flux on the surfaces of the scramjet combustor is very high and dominant, and the convection could not overwhelm the heating effect. In this paper, the convection is to lower the heating rate, and to heat the fuel/coolant as well. The farther of the position from the combustor, the lower of the temperature. The lowest temperature is located at the top left and right corners of the structure, whose boundaries are adiabatic. The highest temperature is located at the position where two surfaces of the combustor cross, and the cooling channel is farther from the position.

In the inverse analysis, the heat flux at the three representative positions in the combustor is assumed unknown and needs to be identified, but everything else is kept the same as in the direct problem. Additional information is the temperature measurements inside the solid structure, which are accessible. In the present work, three positions far from the combustor (near the upper boundary in Fig. 4) are chosen as measurement points, and the measurement is carried out every 10 s. Therefore, there are 60 measurements. It should be addressed here that the identification of convective heat transfer coefficients in regenerative cooling channels is very similar to that of heat flux in this paper.

5.1. Efficiency and accuracy

In this example, the efficiency and the accuracy are to be demonstrated for identifying boundary conditions in the scramjet combustor with the regenerative cooling system. The initial guessed value for each of the heat flux at the three positions is 300 kW/m². Sensitivity analysis is first carried out. Fig. 8 shows the sensitivity coefficients at the first iteration, when the steps for the central format of the finite difference method are 0.01 q₀, 0.06 q₀ and 0.1 q₀. It can be seen that they agree very well with each other, which implies the high accuracy of the central format of the finite difference method for determining sensitivity coefficients in the present work. This is because the direct problem is linear, and the finite difference method is accurate for calculating sensitivity coefficients for linear inverse problems if cancellation errors are not encountered. In the following analysis, the steps for the central format of the FDM are 0.1 q₀.
In this section, the stability for identifying boundary conditions in the scramjet combustor with the regenerative cooling system are examined. Effects of initial guessed values on results are investigated, and another four initial guessed values are tested, 10, 200, 5000 and 10,000, for each inverted parameter. Convergence could be achieved if initial guessed values are 200 and 5000, and convergence curves can be seen in Fig. 10. Divergence occurs when the initial guessed values are 10 and 10,000. This is because the Least-squares method is a gradient-based and local optimum method, and the convergence performance is very dependent on initial guessed values. It can be concluded that the present methodology has a good stability, if initial guessed values do not deviate from real values too much. It can also be seen from Fig. 10 that the iteration numbers are both 5, when initial guessed values are 200 and 5000. In general, the iteration numbers are low, if a convergence could be obtained, even if initial guessed values deviate real values significantly; this further validates the high efficiency for identifying boundary conditions in a scramjet combustor with the regenerative cooling system.

5.3. Effects of measurement errors

In the above analysis, the temperature measurements are exact and without any errors. However, random errors are inevitable in actual measurement. In this example, the effect of the uncertainty of the temperature measurement on the accuracy of the inverse analysis is examined. An error term [50] is added to the exact temperature to account for the random measurement error, which can be seen in Eqs. (10) and (11).

\[
T(x,y,z,t) = T(x,y,z,t)_{\text{exact}} (1 + \zeta_f) \tag{10}
\]

\[
\varphi = \frac{\eta}{2.576} \tag{11}
\]

where \(\zeta\) is the random measurement error, \(\eta\) is a random number between \(-1\) and 1. The value of 2.576 arises from the fact that 99% of a normally distributed population is contained within \pm 2.576 standard deviation of the mean [50].

For quantitatively comparison, relative errors of the identified boundary conditions are defined as:

\[
E_{\text{rel}} = \frac{|q(x,y,z,t)_{\text{identified}} - q(x,y,z,t)_{\text{exact}}|}{q(x,y,z,t)_{\text{exact}}} \times 100\% \tag{12}
\]

Three random measurement errors are considered, i.e., \(\zeta\) is 1%, 3% and 5%, respectively, and the random number distribution is the same for each \(\zeta\). For each measurement error, the convergence could be achieved, and the convergence curves are shown in Fig. 11. It can be seen that only 4, 3 and 5 iterations are required to achieve the convergence, which further validates the high efficiency for identifying boundary conditions in a scramjet combustor with the cooling system. Table 1 lists the identified heat flux, and Table 2 lists the \(E_{\text{rel}}\) values. It can be seen that the identification error increases with the increase of the measurement error, as expected. Moreover, each relative error is very small, which is less than the corresponding measurement error. It means that boundary conditions in a scramjet combustor with a regenerative cooling system could be identified with high accuracy, even with certain measurement errors. The identification is very robust, which is promising in practical applications.

It can be found that the efficiency is very fast from the numerical results, which is attributed to the accurate evaluation of sensitivity coefficients, the high accuracy of the Least-squares method.

6. Conclusions

In this paper, boundary conditions at inaccessible surfaces of a scramjet combustor with the regenerative cooling system are identified by solving a three-dimensional transient inverse heat conduction problem. It is the first time to inversely identify boundary conditions for a scramjet combustor with the regenerative cooling system. The following conclusions can be drawn:

(1) The present methodology is effective, accurate and efficient for inversely identifying boundary conditions in a scramjet combustor with the regenerative cooling system.

(2) The present methodology has a good stability, and initial guessed values only have slight effects on identified results.

(3) The present methodology is robust for identifying boundary conditions in a scramjet combustor with the regenerative cooling system, and boundary conditions could be identified with high accuracy, even with certain measurement errors.

The present methodology is promising in practical engineering applications for determining boundary conditions in a scramjet combustor with a regenerative cooling system.
Fig. 9. Convergence curves of the three parameters of the heat flux with different steps for the FDM for sensitivity analysis (initial guess = 300): (a) 0.01 $q_0$; (b) 0.06 $q_0$; (c) 0.1 $q_0$.

Fig. 10. Convergence curves of the three parameters of the heat flux: (a) initial guess = 200; (b) initial guess = 5000.
Acknowledgments

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References


Table 1
Identified boundary conditions with different measurement errors.

<table>
<thead>
<tr>
<th>Measurement error</th>
<th>Heat flux, kW/m²</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
</tr>
</thead>
<tbody>
<tr>
<td>ζ = 0.0%</td>
<td>460.00</td>
<td>480.00</td>
<td>500.00</td>
<td></td>
</tr>
<tr>
<td>ζ = 1.0%</td>
<td>459.64</td>
<td>480.86</td>
<td>499.88</td>
<td></td>
</tr>
<tr>
<td>ζ = 3.0%</td>
<td>458.91</td>
<td>482.61</td>
<td>499.69</td>
<td></td>
</tr>
<tr>
<td>ζ = 5.0%</td>
<td>458.19</td>
<td>484.36</td>
<td>499.45</td>
<td></td>
</tr>
</tbody>
</table>

Table 2
Relative error $E_{rel}$ of the identified heat flux with different measurement errors.

<table>
<thead>
<tr>
<th>Measurement error</th>
<th>$E_{rel}$ of the identified heat flux, %</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
</tr>
</thead>
<tbody>
<tr>
<td>ζ = 1.0%</td>
<td>0.0780</td>
<td>0.1792</td>
<td>0.0240</td>
<td></td>
</tr>
<tr>
<td>ζ = 3.0%</td>
<td>0.2348</td>
<td>0.5438</td>
<td>0.0620</td>
<td></td>
</tr>
<tr>
<td>ζ = 5.0%</td>
<td>0.3930</td>
<td>0.9080</td>
<td>0.1100</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 11. Convergence curves of the three parameters of the heat flux with different measurement errors: (a) 1%; (b) 3%; (c) 5%.


