Estimation of surface heat flux for ablative material with conjugate gradient method

Qian Wei-qi***, He Kai-feng***, and Zhou Yu*** *State Key Laboratory of Aerodynamics Mianyang Sichuan 621000, China **China Aerodynamics Research and Development Center Mianyang Sichuan 621000, China

Abstract

Estimation of surface heat flux from internal temperature measurements under the circumstances of material ablation is much more complex than the conventional inverse heat conduction problems. In the paper, by utilizing a pyrogeneration-plane ablation model, the conjugate gradient method is developed and verified with numerical examples. And the estimation method is further used to analyze the experimental data of ablation of a Carbon-phenonic material in ceramic-heated tunnel. It is shown that the estimated surface heat flux agrees with the heating power of the tunnel, and the estimation method is basically effective for engineering practices.

1. Introduction

In the reentry process of the hypersonic flight vehicle, the vehicle always suffers extreme thermal loads and the Thermal Protection System(TPS) have to be used to prevent heat from penetrating into the supporting structure of the vehicle. The ablative composite material, such as carbon phenolics and carbon-carbon composites, is the most prevailing-used material of the TPS and the ablation refers to the phenomenon of surface recession of an ablative due to severe thermal attack by an external heat flux. The initial heat transfer into the ablative occurs by pure conduction, and the resulting temperature rise causes material expansion which may be attributed to pure thermal expansion as well as vaporization of any traces of moisture. When the material reaches a sufficiently high temperature, thermochemical degradation or pyrolysis of the material begins. The pyrolysis reactions result in the production of decomposition gases and solid carbonaceous char residue. The thermal expansion and the disappearance of solid material due to the decomposition result in an increase in porosity and permeability of the material. Thus pyrolysis gases begin to escape through the material, removing energy by convention and attenuating the conduction of heat to the reaction zone^[1]. Obviously, under this circumstance, the temperature sensors can only be placed appropriately far from the heated surface in the thermal protection layer and the measured temperature histories are used to estimate the surface heat flux. This is an Inverse Heat Conduction Problem (IHCP) problem^[2,3] and is much more complex than the conventional case because the physics of pyrolysis, charring, and geometry variation have to be taken into account in the estimation algorithm. Due to the complexity, few researches have been carried out about this estimation problem. Kanevce et al.^[4] estimated seven thermal properties of carbon phenolic ablative materials using the Levenberg Marquardt method. Oliveira and Orlande^[5] put forward an algorithm for heat flux estimation of a "non-charring" ablative material using simultaneously temperature measurement as well as measurement of the position of the ablating surface, but in the ablative model, the thermal decomposition of the material is neglected. In ref.[6], an heat flux estimation algorithm based on pyrogeneration-plane ablation model is developed by Hakkaki-Fard and Kowsary and tested with some simulation, but the algorithm is not validated with experimental results. So, in this paper, based on the heat flux estimation method for variable geometry heat conduction problem^[7], the heat flux estimation algorithm also utilizing pyrogeneration-plane ablation model is proposed and validated with ground test data of ceramic-heated tunnel.

2. Ablation model

As mentioned before, the ablation of material is a complex physical and chemical phenomena and for cabonized composite, the pyrogeneration-plane model is adopted as the mathematical model. In this model, the material is

divided into two regions, which are the char layer and the virgin material (Fig.1), and the pyrolysis zone is simplified to be a surface connecting the two regions. The two moving boundaries, char and pyrolysis boundaries and a constant boundary are defined as " s_1 ", " s_2 " and " s_3 "in Fig.1. The control equations for this model are,



Figure 1: Pyrogeneration-plane ablation model

$$\begin{cases} \frac{\partial}{\partial x} \left[k_c \frac{\partial T}{\partial x} \right] + \dot{m}_p c_g \frac{\partial T}{\partial x} = \rho_c c_c \frac{\partial T}{\partial t}; \quad x \in (s_1(t), s_2(t)) \\ \frac{\partial}{\partial x} \left[k_v \frac{\partial T}{\partial x} \right] = \rho_v c_v \frac{\partial T}{\partial t}; \quad x \in (s_2(t), s_3(t)) \\ T(x,0) = T_0 \\ -k_c \frac{\partial T}{\partial x} = Q(t); \quad x = s_1(t) \\ -k_c \frac{\partial T}{\partial x} = -k_v \frac{\partial T}{\partial x} + \dot{m}_p \Delta H_p; \quad x = s_2(t) \\ k_v \frac{\partial T}{\partial x} = 0; \quad x = s_3(t) \end{cases}$$
(1)
and $s_1(t) = \int_0^t \frac{\dot{m}_c}{\rho_1} dt; \quad s_2(t) = \int_0^t \frac{\dot{m}_p}{\rho_2 - \rho_1} dt.$

where the subscripts of "c", "v", "g" denote the char layer, the virgin material, and the gases from pyrolysis respectively; \dot{m}_p is the specific pyrolysis mass flow rate; \dot{m}_c is the specific ablation mass flow rate; ΔH_p is the specific pyrolysis heat; and the term of $\dot{m}_p c_g \frac{\partial T}{\partial x}$ is the ventilation influence of the pyrolysis gas.



Figure 2: Sketch of finite control volume

In this paper, FCV(Finite Control Volume) method^[2] is applied for solving the Eqs.(1), and the typical control volume is sketched in Fig 2, 'i-1', 'i', 'i+1' denoting the grid nodes, the shaded area being the control volume of the FCV. Moreover, because the boundary positions of $s_1(t)$ and $s_2(t)$ moves timely, the semi-discrete form of energy equation for this control volume in the FCV is different from the fixed geometry conditions, being of the following form,

$$k\frac{\partial T}{\partial x}\Big|_{w}^{e} + (\rho C_{p}Tu)_{e} - (\rho C_{p}Tu)_{w} = \left[\frac{d}{dt}\left(\int_{w}^{e} \rho C_{p}Tdx\right)\right]$$
(2)

in which *u* denote the translational speed and the last two terms on the left side of this equation are the net enthalpy flux into the control volume resulting from control volume boundary translation. So, When the functions of $s_1(t)$ and $s_2(t)$ are given by measurement or decided by iterative calculation to meet the given temperature of ablation and pyrolysis surface, the right boundary is assumed to be adiabatic, the direct heat conduction problem of Eqs.(1) can be solved numerically. The correctness of modified FCV has been verified by solving the following heat conduction problem with analytical solution^[8].

3. Inverse Problem

For direct heat conduction problem, when the heat flux Q(t) is specified, the temperature field of T(x,t) and ablation variables can be solved. Now if the heat flux Q(t) is unknown and the temperature histories at some measurement position x_m are measured, it turns out to be a typical IHCP problem of surface heat flux estimation. This IHCP often can be solved with optimization method, i.e., finding a heat flux profile that minimizes the difference between the measurement and the estimated temperature. Here, without losing generalization, the measurement position is chosen as the right boundary, then the objective function can be written as,

$$J = \int_0^{t_f} \left[T(s_3, t, Q) - \tilde{T}(s_3, t) \right]^2 dt$$
(3)

where $T(s_3, t, Q)$ is computed temperature at the measurement location from Eqs.(1) with a heat flux function of Q, and $\tilde{T}(s_3, t)$ is measured temperature history at right boundary, and $[0, t_f]$ is the time interval.

In order to solve this optimization problem, Eqs.(1) is multiplied by the Lagrange multiplier (or adjoint function) λ and added to Eq.(3) to get the following expression,

$$J = \int_{0}^{t_{f}} \left[T(s_{3}, t, Q) - \widetilde{T}(s_{3}, t, Q) \right]^{2} dt + \int_{0}^{t_{f}} \int_{s_{1}(t)}^{s_{2}(t)} \left(\frac{\partial}{\partial x} \left[k_{c} \frac{\partial T}{\partial x} \right] + \dot{m}_{p} c_{g} \frac{\partial T}{\partial x} - \rho_{c} c_{c} \frac{\partial T}{\partial t} \right) \lambda(x, t) dx dt + \int_{0}^{t_{f}} \int_{s_{2}(t)}^{s_{3}(t)} \left(\frac{\partial}{\partial x} \left[k_{v} \frac{\partial T}{\partial x} \right] - \rho_{v} c_{v} \frac{\partial T}{\partial t} \right) \lambda(x, t) dx dt$$
(4)

After integrating by parts and doing the variational analysis, we can get

$$\delta J = \int_{0}^{t_{f}} 2[T(s_{3},t,Q) - \widetilde{T}(s_{3},t)]\Delta T dt$$

$$+ \int_{0}^{t_{f}s_{2}(t)} \left(k_{c} \frac{\partial^{2} \lambda}{\partial x^{2}} - \dot{m}_{p}c_{g} \frac{\partial \lambda}{\partial x} + \rho_{c}c_{c} \frac{\partial \lambda}{\partial t}\right)\Delta T dx dt dx dt + \int_{0}^{t_{f}s_{3}(t)} \left(k_{v} \frac{\partial^{2} \lambda}{\partial x^{2}} + \rho_{v}c_{v} \frac{\partial \lambda}{\partial t}\right)\Delta T dx dt$$

$$+ \int_{0}^{t_{f}} \Delta T(k_{c} \frac{\partial \lambda}{\partial x} - \dot{m}_{p}c_{g}\lambda - \rho_{c}c_{c}\lambda \frac{dx}{dt})\Big|_{x=s_{1}(t)} dt - \int_{0}^{t_{f}} \Delta T(k_{v} \frac{\partial \lambda}{\partial x} - \rho_{v}c_{v}\lambda \frac{dx}{dt})\Big|_{x=s_{3}(t)} dt$$

$$- \int_{0}^{t_{f}} \Delta T\Big[(k_{c} \frac{\partial \lambda}{\partial x} - \dot{m}_{p}c_{g}\lambda - \rho_{c}c_{c}\lambda \frac{dx}{dt}) - (k_{v} \frac{\partial \lambda}{\partial x} - \rho_{v}c_{v}\lambda \frac{dx}{dt})\Big]_{x=s_{2}(t)} dt$$

$$- \int_{0}^{t_{f}} (\Delta Q\lambda)\Big|_{x=s_{1}(t)} dt - \int_{s_{2}(t_{f})}^{s_{3}(t_{f})} \rho_{v}c_{v}(\Delta T\lambda)\Big|_{t=t_{f}} dx - \int_{s_{2}(t_{f})}^{s_{3}(t_{f})} \rho_{c}c_{c}(\Delta T\lambda)\Big|_{t=t_{f}} dx$$
(5)

By considering the arbitrariness of the ΔT value and applying variational principle, the equation for the adjoint function can be deduced as

$$k_{c}\frac{\partial^{2}\lambda}{\partial x^{2}} - \dot{m}_{p}c_{g}\frac{\partial\lambda}{\partial x} + \rho_{c}c_{c}\frac{\partial\lambda}{\partial t} = 0; \quad x \in (s_{1}(t), s_{2}(t))$$

$$k_{v}\frac{\partial^{2}\lambda}{\partial x^{2}} + \rho_{v}c_{v}\frac{\partial\lambda}{\partial t} = 0; \quad x \in (s_{2}(t), s_{3}(t))$$

$$\lambda(x, t_{f}) = 0$$

$$k_{c}\frac{\partial\lambda}{\partial x} - \dot{m}_{p}c_{g}\lambda - \rho_{c}c_{c}\lambda\frac{ds_{1}}{dt} = 0; \quad x = s_{1}(t)$$

$$(k_{c}\frac{\partial\lambda}{\partial x} - \dot{m}_{p}c_{g}\lambda - \rho_{c}c_{c}\lambda\frac{ds_{2}}{dt}) = (k_{v}\frac{\partial\lambda}{\partial x} - \rho_{v}c_{v}\lambda\frac{ds_{2}}{dt}); \quad x = s_{2}(t)$$

$$k_{v}\frac{\partial\lambda}{\partial x} - \rho_{v}c_{v}\lambda\frac{ds_{3}}{dt} = 2[T(s_{3}, t) - \widetilde{T}(s_{3}, t)]; \quad x = s_{3}(t)$$
(6)

and the gradient of objective function with respect to Q is

$$\frac{\partial J}{\partial Q}(t) = -\lambda(s_1, t) \tag{7}$$

Based on this gradient, the steepest descent method or the conjugate gradient method(CGM) can be used to carry out the parameter optimization. In this paper, the CGM is utilized, the optimization algorithm is^{[3][9]},

$$Q_{i}^{l+1} = Q_{i}^{l} - \beta^{l} \left(S_{i}\right)^{l}; \left(S_{i}\right)^{l} = J^{\prime l} + \gamma^{l} \left(S_{i}\right)^{l-1}; J^{\prime l} = \left(\frac{\partial J}{\partial Q_{i}}\right)^{l};$$

$$\gamma^{l} = \int_{t=0}^{t_{f}} \left(J^{\prime l}\right)^{2} dt / \int_{t=0}^{t_{f}} \left(J^{\prime l-1}\right)^{2} dt; \beta^{l} = \int_{t=0}^{t_{f}} \left\{ \left[T(s_{3},t) - \widetilde{T}(s_{3},t)\right] U(s_{3},t) \right\} dt / \int_{t=0}^{t_{f}} \left[U(s_{3},t)\right]^{2} dt$$
(8)

where the superscripts of *l*, *l*+1 denote the iteration level of optimization, β^{l} is the search step size, the subscript of *i* denotes the discretized time level, and *U* is the sensitivity of temperature field change aroused by letting $\Delta Q = (S_i)^{l}$. i.e. using the difference method,

$$U(s_{3},t) = T(s_{3},t,Q + \Delta Q) - T(s_{3},t,Q); \text{ and } \Delta Q_{i} = (S_{i})^{l}$$
(9)

Finally, the following criterion for J is used to stop the optimization of Eq.(8),

$$J \le \delta, \ \delta = \sigma^2 t_f \tag{10}$$

where σ is the standard deviations of measurement noise.

4. Example test

The aforementioned estimation method is verified with a numerical example at first. In this test case, the thermophysical parameters are set as $\rho_v=1300$ kg/m³, $c_v=1507$ J/kgK, $k_v=1$ W/(mK), $\rho_c=406.3$ kg/m³, $c_c=2000$ J/kgK, $k_c=3$ W/(mK), $C_g=1300$ J/kgK, $\Delta H_p=831500$ J/kg, the temperature of pyprolysis is 873K and initial thickness of the material L is 20mm.

The surface heat flux and ablated surface position of $s_1(t)$ are specified as "Qexact" in Fig.3 and Fig.4, then Eqs.(1) can be solved with FCV and the temperature history at the measurement position is obtained. In the solving process, the pyrolysis position of $s_2(t)$ is iteratively determined by the constraint that the calculated temperature at the position is equal to the given temperature of pyrolysis. The calculated position now is shown in Fig.5.

In order to validate the effectiveness of the estimation algorithm, the calculated temperature history on measurement locations is used as measurement data to estimate the heat flux at first. The estimated result is shown as the dashed line("Qestimated($\sigma=0K$)") in Fig.3, agreeing with the specified heat flux well except for the final time. The difference may be due to the reason that the influence of surface heat flux at the final time can not be conducted to

the measurement point which is a bit far from the heating surface and its information can not be reflected from the simultaneous temperature history at the measurement point.



Figure 3: Comparison of exact and estimated value of heat flux



Figure 4: Time history of ablated surface recession



Figure 5: Time history of calculated pyrogeneration-plane



Figure 6: Comparison of temperature measurement

Because the measurement noise is unavoidable and play an important role on the accuracy of the estimated result, the calculated temperatures at measurement locations with exact surface heat flux are now added with some white noise whose standard deviations is σ =6K, about 1% relative error to the maximum temperature increase, to simulate the measurement data, shown as "Exp." in Fig.6. The estimated result is shown as "Qestimated(σ =6K)" in Fig.3, also agreeing with the specified heat flux well, and the calculated temperature history at the measurement position with the estimated heat flux, shown as "Fitted" in Fig.6, fits the measurement data. And when the measurement noise is increased from σ =6K to σ =12K, the estimated result deviates more from the specified heat flux, but still reflecting the pattern and magnitude of the heat flux generally, which is shown as "Qestimated(σ =12K)" in Fig.3. The results exhibit that the estimation method is feasible and not very sensitive to the measurement noise.



Figure7: Experimental results of blunt Carbon-phenonic material ablation

5. Ground test result estimation

Furthermore, the estimation method is applied for the experimental data of a ground test. A piece of blunt model made of Carbon-phenonic material Narmco is tested in the ceramic-heated tunnel of NASA Langley center^[10]. The temperature at the ablated surface, the ablated and pyrolysis boundaries are measured and given as "Front surface" and "Interface" in Fig.7. With these measurement data, the surface heat flux can be estimated with the method developed in this work and shown as "Estimated Q" in Fig.8, and it is found that the estimated surface heat flux is close to the heating power value of the ceramic-heated tunnel. This result shows that the estimation method developed in this paper is preliminarily validated with practical experimental data and the method is basically effective to treat the heat conduction problem with ablation.



Figure 8: Comparison of estimated heat flux and electrical heating power

6. Conclusion

In this paper, the CGM along with the associated adjoint problem is developed to estimate the heat flux at the surface of an ablative material. Results for noise-free and noisy simulated measurement data show that the estimation method employing the pyrogeneration-plane ablation model is feasible and robust. The larger is the measurement noise, the greater is the deviation of the estimated result from the exact value. The estimation method is further practically applied to analyze the ablation test data of a blunt Carbon-phenonic Narmco4028 material in the ceramic-heated tunnel, and the agreement between the estimated heat flux and the electrical heating power shows that the estimation method is basically effective to treat the engineering heat conduction problem with ablation. With more examples' verification and validation the estimation method may exhibit a good potentiality of application in future flight practices.

Acknowledgements

The authors are grateful for the support provided by the National Natural Science Foundation of China (Grant No.11372338) and the foundation of the State Key Laboratory of Aerodynamics (Grant No.JBKY11030903).

References

- [1] Jiang, G. Q., and L. Y. Liu. 2003. Heat transfer of hypersonic gas and ablation thermal protection. National Defense Industrial Press, Beijing. (In Chinese)
- [2] Beck, J. V., Blackwell, B. and C. R. S. Jr Clair. 1985. Inverse heat conduction-ill-posed problems. John Wiley&Sons, New York.
- [3] Alifanov, O. M. 1994. Inverse heat transfer problems. Springer-Verlag, Berlin.
- [4] Kanevce, L. P., Kanevce, G. H., and Z. Z. Angelevski. 1999. Comparison of two kinds of experiments for estimation of thermal properties of ablative composite. In: *Inverse Problems in Engineering: Theory and Practice-3rd Int. Conference on Inverse Problems in Engineering*. EXP01, 1-7.
- [5] Oliveira, A. P. D., and H. R. B. Orlande. 2004. Estimation of the heat flux at the surface of ablating materials by using temperature and surface position measurements. *Inverse Problems in Science and Engineering*. 12(5):563-577.
- [6] Hakkaki-Fard, A., and F. Kowsary. 2008. Heat flux estimation in a charring ablator. *Numerical Heat Transfer, Part A*. 53:543-560.
- [7] He, K. F., Qian, W. Q., Zhou, Y., and Y. P. Shao. 2013. Estimation of surface heat flux for variable geometry heat conduction problem. In: *IPDO2013-4th Inverse problems, Design and Optimization symposium*. 55-56.
- [8] Shao Y. P., Qian, W. Q., Zhou, Y., Yang C., and J. D. Huang. 2013. Estimation of surface heat flux for variable geometry inverse heat conduction problem. *Chinese Journal of Computational Mechanics*. 30(2):296-301. (In Chinese)
- [9] Qian, W. Q., Zhou, Y., He, K. F., Yuan, J. Y., and J. D. Huang. 2012. Estimation of surface heat flux for nonlinear inverse heat conduction problem. *ACTA AERODYNAMICA SINICA*. 30(2):145-150. (In Chinese)
- [10] Sutton, K. 1970. An experimental study of a carbon-phenolic ablation material. NASA-TND-5930. NASA.