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Shape optimization of thermo-diffusive systems

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Abstract—A method of design sensitivity analysis for shape optimization of a thermo-diffusive system is developed. In the method an optimization problem is defined in functional form. The material derivative concept and an adjoint variable method are employed for the shape design sensitivity analysis. An axisymmetric problem of thermo-diffusion is an illustration of the method presented.

INTRODUCTION

IN THE present paper, a general method of design sensitivity analysis for shape optimal design of thermo-diffusive systems is developed. In the method an optimization problem is defined in functional form. The material derivative idea and an adjoint variable method are employed for shape design sensitivity analysis. The state and adjoint system equations are finally formulated. In the paper, the material properties and thermal loads of a thermo-diffusive system are held fixed, while the domain shape is varied in order to meet some desired physical objectives. Shape optimization of thermo-diffusive systems has not been undertaken in the literature. The material derivative concept has been successfully applied to variational problems on varying domains in structural optimization problems by several authors [1–5]. Much literature is available on structural shape optimization problems involving mechanical effects only. However, few structural optimization studies under the influence of temperature have appeared in the literature [5–7]. Most of these works are analyzed on fixed domains by incorporating the design variables or parameters into the governing equations. In the present study the shape configuration of the domain is adopted as the decision variable. The shape sensitivity analysis of an integral functional, representing the system's response of interest, for a thermo-diffusive system is accomplished by the adjoint variable method and material derivative concept. The shape sensitivity analysis expressions, which are defined only on the varying portions of the boundary, may then be employed for any shape optimization or identification problem at hand. References [8–10] provide general information on functional analysis and variational methods used in this work.

THERMO-DIFFUSIVE EQUATIONS

In our analysis we consider a thermo-diffusive system in the domain Ω governed by the equations

$$-q_{i,i}+Q = 0, \tag{1}$$

$$u_{k,ii}+g\beta T\gamma_k = 0, \tag{2}$$

$$u_{k,k} = 0, \tag{3}$$

where Ω is the domain to be varied, q_i is the heat flux vector, u_k is the velocity component, g is the acceleration due to gravity, β is the coefficient of volumetric thermal expansion, T is the temperature, γ_k is the unit vector component and Q is the distributed heat source.

Equation (2) can be written as

$$u_{k,ii}+b_k = 0 \tag{4}$$

where

$$b_k = g\beta T\gamma_k.$$

For thermal problems, the boundary conditions can be expressed as

$$T = T^{\mathrm{b}} \quad \text{on} \quad \partial\Omega_T, \tag{5}$$

$$q = q^{\mathrm{b}} \quad \text{on} \quad \partial\Omega_q, \tag{6}$$

where q is the heat flux normal to the boundary. For a velocity field the boundary conditions are as follows:

$$u_i = u_i^{\mathrm{b}} \quad \text{on} \quad \partial\Omega_u \tag{7}$$

$$t_i = t_i^{\mathrm{b}} \quad \text{on} \quad \partial\Omega_t \tag{8}$$

where $t_i = u_{i,j}n_j$ and n_j is the normal to the boundary. Moreover, we have the relation

$$q_i = -kT_{,i} \tag{9}$$

where k is the thermal conductivity.

SHAPE SENSITIVITY ANALYSIS

In our approach to shape optimization, the material characteristics and loading functions are all given quantities. However, the shape configuration of the domain Ω and its boundary surface $\partial\Omega$ is not given a priori in the problem. The domain shape will be taken as the decision variable itself so as to satisfy some physical objectives having desired distributions of temperature, velocity, etc. A general integral functional will be adopted that may serve as the objective function to be extremized, or a behavioral constraint to be satisfied in a shape optimization problem. This functional, which is termed as the general performance criterion Λ, is defined in the domain Ω and the boundary $\partial\Omega$ as follows:

$$\Lambda = \int_\Omega r(T, q_i, u_k, u_{k,i})\, \mathrm{d}\Omega + \int_{\partial\Omega} s(T, q, u_k, t_k)\, \mathrm{d}(\partial\Omega). \tag{10}$$

The shape sensitivity analysis may now be stated to find the total variation of Λ with respect to variations in the domain Ω subject to the primary problem equations (1)–(9).

In the so-called adjoint variable method of optimization, equilibrium equations are incorporated into the general performance criterion Λ in terms of the adjoint temperature T^* and velocity u^*

$$\bar{\Lambda} = \Lambda + \int_\Omega (T^*(-q_{i,i} + Q) + u_k^*(u_{k,ii} + b_k))\, \mathrm{d}\Omega \tag{11}$$

where $\bar{\Lambda}$ is the augmented functional. Integration by parts gives

$$\bar{\Lambda} = \int_\Omega (r + q_i T^*_{,i} + QT^* - u_{k,i}u^*_{k,i} + b_k u_k^*)\, \mathrm{d}\Omega + \int_{\partial\Omega} (s - qT^* + t_k u_k)\, \mathrm{d}(\partial\Omega). \tag{12}$$

The shape of domain Ω, being the decision variable itself, is not fixed. This variation of Ω under a transformation is characterized by a time-like parameter τ. Thus following refs. [1–5], a point x_i in Ω (at $\tau = 0$) moves to the point x_i^τ in the varied domain Ω^τ under the transformation $\eta: x_i \to x_i^\tau,\ x_i \in \Omega$ given by

$$x_i^\tau = \eta(x_i, \tau) + \tau V_i(x_j) \tag{13}$$

$$\Omega^\tau = \eta(\Omega, \tau) \tag{14}$$

where V_i is the deformation velocity field which represents the rate of domain deformation (see Fig. 1). Thinking of τ as the time variable, the material derivative of a continuously differentiable function w is defined as

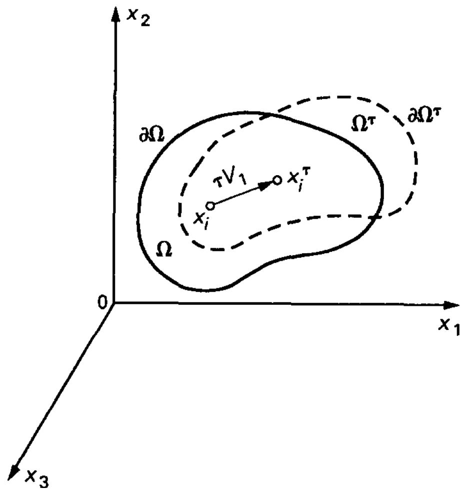

FIG. 1. Domain Ω undergoing deformation velocity V_i.

$$\dot{w} = w' + w_{,k} V_k \tag{15}$$

where ($\dot{}$) and ( )$'$ denote the material and partial derivatives of ( ) respectively with respect to τ.

Since the augmented functional $\bar{\Lambda}$ is described by integrals, the material derivative of general domain and surface integrals will also be given as follows [1, 3]:

$$\varphi_1 = \int_\Omega w_1\, \mathrm{d}\Omega \quad \dot{\varphi}_1 = \int_\Omega w_1'\, \mathrm{d}\Omega + \int_{\partial\Omega} w_1 V_n\, \mathrm{d}(\partial\Omega) \tag{16}$$

$$\varphi_2 = \int_{\partial\Omega} w_2\, \mathrm{d}(\partial\Omega)$$

$$\dot{\varphi}_2 = \int_{\partial\Omega} (w_2' + (w_{2,n} + Hw_2)V_n)\, \mathrm{d}(\partial\Omega) \tag{17}$$

where ( )$_{,n}$ indicates the normal derivative of ( ), H is the curvature of the boundary $\partial\Omega$ and V_n is the normal component of the deformation velocity V_i given by $V_n = V_i n_i$.

Using (16) and (17), the material derivative of $\bar{\Lambda}$ may be given in the following form:

$$\dot{\bar{\Lambda}} = \int_\Omega \left(\frac{\partial r}{\partial T} T' + \frac{\partial r}{\partial q_i} q_i' + \frac{\partial r}{\partial u_k} u_k' + \frac{\partial r}{\partial u_{k,i}} u_{k,i}' + q_i T^{*\prime}_{,i} + T^*_{,i} q_i' + QT^{*\prime} - u_{k,i} u^{*\prime}_{k,i} - u^*_{k,i} u'_{k,i} + b_k u_k^{*\prime} + b_k' u_k^* \right) \mathrm{d}\Omega + \int_{\partial\Omega} \left((r + q_i T^*_{,i} + QT^* - u_{k,i} u^*_{k,i} + b_k u_k^* + (s - qT^* + t_k u_k^*)_{,n} + H(s - qT^* + t_k u_k^*))V_n + \frac{\partial s}{\partial T} T' + \frac{\partial s}{\partial q} q' + \frac{\partial s}{\partial u_k} u_k' + \frac{\partial s}{\partial t_k} t_k' - qT^{*\prime} - T^* q' + t_k u_k^{*\prime} + u_k^* t_k' \right) \mathrm{d}(\partial\Omega). \tag{18}$$

By (9) and (4) we get respectively

$$q_i' = -kT_{,i}' \tag{19}$$

$$b_k' = g\beta\gamma_k T'. \tag{20}$$

Integrating (18) by parts again and using (19) and (20) we obtain

$$\begin{aligned}\dot{\Lambda} = \int_\Omega \Bigg(& (-q_{i,i}+Q)T^{*\prime} + (u_{k,ii}+b_k)u_k^{*\prime} \\ & + \left(-\hat{q}_{i,i}^* + g\beta\gamma_k u_k^* + \frac{\partial r}{\partial T}\right)T' \\ & + \left(\hat{u}_{k,ii} + \frac{\partial f}{\partial u_k}\right)u_k'\Bigg)\,\mathrm{d}\Omega + \int_{\partial\Omega}\Bigg((r+q_i T_{,i}^* \\ & + QT^* - u_{k,i}u_{k,i}^* + b_k u_k^* + (s-qT^*+t_k u_k^*)_{,\mathrm{n}} \\ & + H(s-qT^*+t_k u_k^*))V_\mathrm{n} + \left(\frac{\partial s}{\partial T} + \hat{q}^*\right)T' \\ & + \left(\frac{\partial s}{\partial u_k} - \hat{t}_k^*\right)u_k' + \left(\frac{\partial s}{\partial q} - T^*\right)q' \\ & + \left(\frac{\partial s}{\partial t_k} + u_k^*\right)t_k'\Bigg)\,\mathrm{d}(\partial\Omega) \end{aligned} \tag{21}$$

where the adjoint variables $\hat{q}_i^*$ and $\hat{u}_{k,i}^*$ are defined by

$$\hat{q}_i^* = -k\left(T_{,i}^* + \frac{\partial r}{\partial q_i}\right) \tag{22}$$

$$\hat{u}_{k,i}^* = \left(-u_{k,i}^* + \frac{\partial r}{\partial u_{k,i}}\right) \tag{23}$$

and the adjoint variables $\hat{q}^*$ and $\hat{t}_k^*$ are given by

$$\hat{q}^* = \hat{q}_i^* n_i \tag{24}$$

$$\hat{t}_i^* = \hat{u}_{k,i} n_i. \tag{25}$$

The partial derivative of the boundary conditions with respect to τ can now be derived from equations (5)–(8).

Based on (15) we have

$$\dot{T} = \dot{T}^\mathrm{b} \quad \text{on} \quad \partial\Omega_T \tag{26}$$

and

$$T' + T_{,k}V_k = T^{\mathrm{b}\prime} + T_{,k}^\mathrm{b} V_k. \tag{27}$$

Since $T^{\mathrm{b}\prime} = 0$ we get

$$T' = (T_{,k}^\mathrm{b} - T_{,k})V_k. \tag{28}$$

Similarly we obtain

$$q' = (q_{,k}^\mathrm{b} - q_{,k})V_k \quad \text{on } \partial\Omega_q \tag{29}$$

$$u_k' = (u_{k,i}^\mathrm{b} - u_{k,i})V_i \quad \text{on } \partial\Omega_u \tag{30}$$

$$t_k' = (t_{k,i}^\mathrm{b} - t_{k,i})V_i \quad \text{on } \partial\Omega_t. \tag{31}$$

In order to get rid of the terms involving partial derivatives with respect to τ in $\dot{\Lambda}$ it is now required that the following adjoint problem is satisfied:

$$-\hat{q}_{i,i}^* + g\beta\gamma_k u_k^* + \frac{\partial r}{\partial T} = 0 \quad \text{in } \Omega \tag{32}$$

$$\hat{u}_{k,ii} + \frac{\partial f}{\partial u_k} = 0 \quad \text{in } \Omega \tag{33}$$

$$T^* = \frac{\partial s}{\partial q} \quad \text{on } \partial\Omega_T \tag{34}$$

$$q^* = -\frac{\partial s}{\partial T} \quad \text{on } \partial\Omega_q \tag{35}$$

$$u_k^* = -\frac{\partial s}{\partial t_k} \quad \text{on } \partial\Omega_u \tag{36}$$

$$t_k^* = \frac{\partial s}{\partial u_k} \quad \text{on } \partial\Omega_t. \tag{37}$$

If the primary problem, equations (1)–(9), and the adjoint problem, equations (22), (23) and (32)–(37), are satisfied for an instantaneous domain Ω at $\tau = 0$, the total variation of Λ is given by the following expression:

$$\begin{aligned}\dot{\Lambda} = \int_{\partial\Omega} & (r + q_i T_{,i}^* + QT^* - u_{k,i}u_{k,i}^* + b_k u_k^* \\ & + (s-qT^*+t_k u_k^*)_{,\mathrm{n}} + H(s-qT^* \\ & + t_k u_k^*))V_\mathrm{n}\,\mathrm{d}(\partial\Omega) \\ & + \int_{\partial\Omega_T}\left(\frac{\partial s}{\partial T} + \hat{q}^*\right)(T_{,k}^\mathrm{b} - T_{,k})V_k\,\mathrm{d}(\partial\Omega) \\ & + \int_{\partial\Omega_q}\left(\frac{\partial s}{\partial q} - T^*\right)(q_{,k}^\mathrm{b} - q_{,k})V_k\,\mathrm{d}(\partial\Omega) \\ & + \int_{\partial\Omega_u}\left(\frac{\partial s}{\partial u_k} - \hat{t}_k^*\right)(u_{k,i}^\mathrm{b} - u_{k,i})V_i\,\mathrm{d}(\partial\Omega) \\ & + \int_{\partial\Omega_t}\left(\frac{\partial s}{\partial t_k} + u_k^*\right)(t_{k,i}^\mathrm{b} - t_{k,i})V_i\,\mathrm{d}(\partial\Omega). \end{aligned} \tag{38}$$

It should be noted that in order to evaluate the material derivative of $\dot{\Lambda}$, the coupled primary and adjoint equations must be solved in the following order:

the T problem given in equations (1), (5), (6) and (9);
the u_k problem given in equations (2), (3), (7) and (8);
the u_k^* problem given by equations (23), (33), (36) and (37);
the T^* problem given by equations (22), (32), (34) and (35).

EXAMPLE

For a fully 3D thermo-diffusive system the primary and adjoint problems as well as boundary surfaces must usually be discretized by using finite elements or boundary elements in order to obtain the variation of performance criterion with respect to domain variations. In the present study only the one-dimensional shape optimization problem in which analytical expressions for the field variables can be obtained will be analyzed.

Consider the axisymmetric problem of a fixed inner radius r_1 and an outer radius r_2 which is to be optimized and subject to thermal surface conditions (Fig. 2). The problem is described as

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right)+g\beta T=0 \tag{39}$$

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right)=0 \tag{40}$$

$$\operatorname{div} u=0 \tag{41}$$

$$u_{r=r_1}=0 \tag{42}$$

$$u_{r=r_2}=0 \tag{43}$$

$$T_{r=r_1}=T_1 \tag{44}$$

$$T_{r=r_2}=T_2. \tag{45}$$

The outer radius r_2 will be optimally chosen such that the independent objective function J is maximized

$$\text{maximize } J=\text{ABS}\left|u\left(\frac{r_1+r_2}{2}\right)\right|. \tag{46}$$

The adjoint problem is defined by the following:

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du^*}{dr}\right)=0,\quad \frac{1}{r}\frac{d}{dr}\left(r\frac{dT^*}{dr}\right)-g\beta u^*=0.$$

The following parameters are assumed: $r_1=10$, $g=1$, $\beta=1$ with assumptions of two cases:

1st $\quad T_1=5,\quad T_2=2$

2nd $\quad T_1=2,\quad T_2=5.$

Figure 3(a) presents the absolute value of velocity

$$\left|u\left(\frac{r_1+r_2}{2}\right)\right|$$

as a function of r_2 for the first case and Fig. 3(b) for the second one. Figures 4 and 5 analyze distributions of velocity $|u|$ and temperature T for the optimal radii obtained. In each case, starting from an initial guess for the outer radius r_2, the primary and adjoint variables may be obtained numerically. The maximization of the objective function J can then be obtained by using its functional value and its gradient with respect to the corresponding decision parameter via a numerical maximization scheme. It is, of course, possible to obtain the optimal solution for r_2 corresponding to the objective function J by simply differentiating it with respect to r_2. However, the optimal r_2 is calculated via the general shape sensitivity analysis presented in this study.

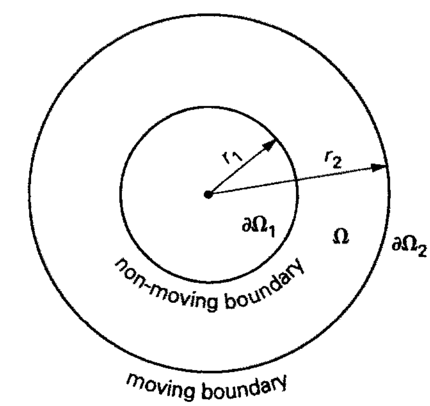

FIG. 2. Scheme of axisymmetric thermo-diffusive system with moving boundary $\partial\Omega_2$.

FINAL REMARKS

Utilizing the sensitivity analysis, a method of shape design sensitivity analysis is established through a systematic method of constructing adjoint equations. The method finds an application in the process of various thermo-diffusive systems. The derivation of the general sensitivity expressions has been performed without regard to any specific shape, and hence the results apply to any regular space geometries. It

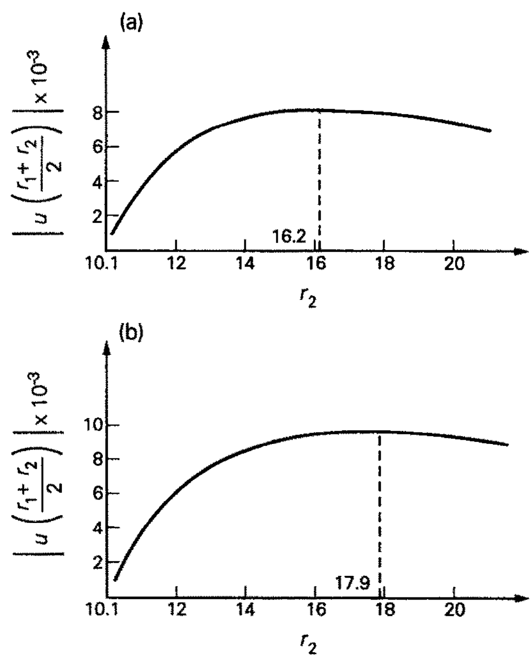

FIG. 3. Absolute value of the velocity in the middle of the tube as a function of r_2. (a) $T_1=5$, $T_2=2$. (b) $T_1=2$, $T_2=5$.

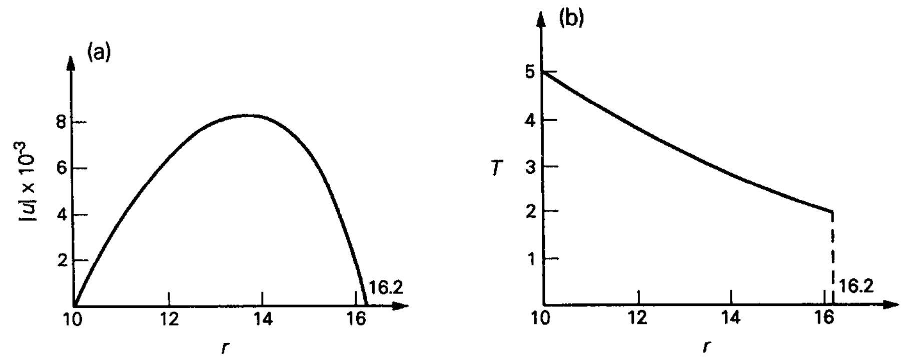

FIG. 4. Absolute value of velocity (a) and temperature (b) in the tube for optimal radius $r_2 = 16.2$, $T_1 = 5$ and $T_2 = 2$.

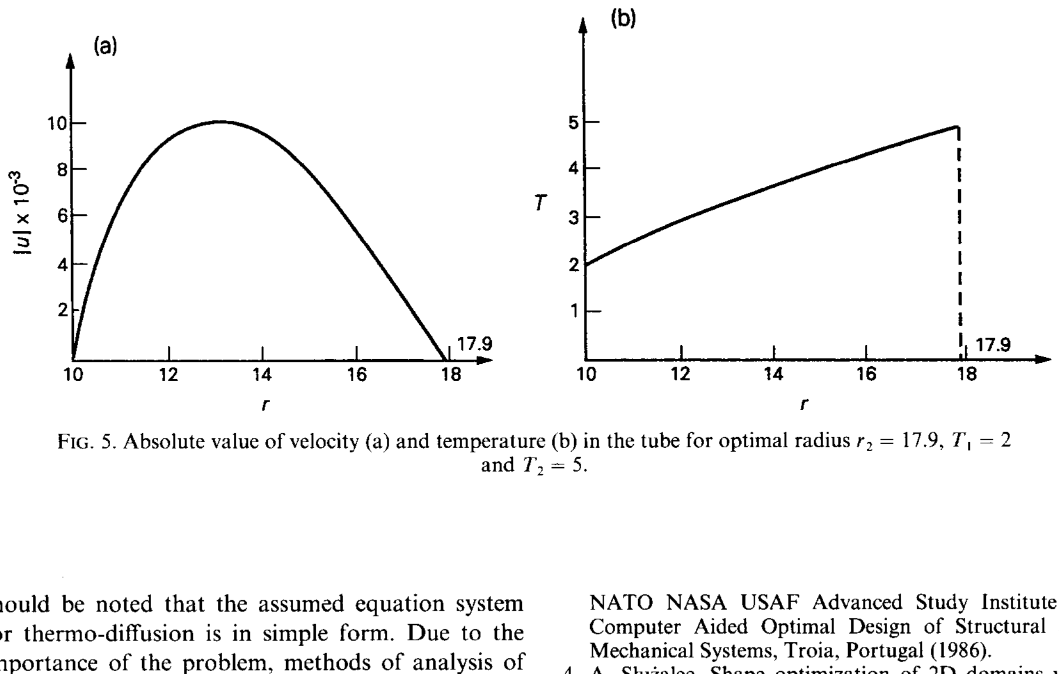

FIG. 5. Absolute value of velocity (a) and temperature (b) in the tube for optimal radius $r_2 = 17.9$, $T_1 = 2$ and $T_2 = 5$.

should be noted that the assumed equation system for thermo-diffusion is in simple form. Due to the importance of the problem, methods of analysis of more complicated forms of thermo-diffusion equations, which can be used in the processes of optimization, should be undertaken.

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OPTIMISATION DE LA FORME DES SYSTEMES THERMO-DIFFUSIFS

Résumé—On développe une méthode d'analyse de sensibilité pour l'optimisation de la forme d'un système thermo-diffusif. Un problème d'optimisation est défini sous forme fonctionnelle. Le concept de dérivée matérielle et une méthode de variable adjointe sont employés pour l'analyse de sensibilité à la conception de la forme. On présente, en illustration, un problème axisymétrique de thermodiffusion.

FORM-OPTIMIERUNG THERMO-DIFFUSIVER SYSTEME

Zusammenfassung—Es wird ein Verfahren für die Sensitivitätsanalyse zur Formoptimierung eines thermodiffusiven Systems entwickelt. Bei diesem Verfahren wird ein Optimierungsproblem in funktionaler Form definiert. Bei der Formsensitivitätsanalyse wird das vom Material abgeleitete Konzept und ein Verfahren der variablen Anpassung angewandt. Abschließend wird die Vorgehensweise anhand eines achsensymmetrischen Problems der Thermo-Diffusion verdeutlicht.

ОПТИМИЗАЦИЯ ФОРМЫ ТЕРМОДИФФУЗИОННЫХ СИСТЕМ

Аннотация—Разработан метод анализа расчетной чувствительности для оптимизации формы термодиффузионных систем. Задача оптимизации определяется в функциональном виде. В анализе используются производный подход к материалу и взаимосвязанный метод переменных. Использование предложенного метода иллюстрируется на примере осесимметричной задачи термодиффузии.