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A sensitivity analysis for the determination of unknown thermal coefficients through a phase-change process with temperature-dependent thermal conductivity ☆

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ABSTRACT

In Tarzia, Int. Comm. in Heat and Mass Transfer, 25 (1998), 139–147, explicit formulas for the simultaneous determination of unknown thermal coefficients of a semi-infinite material through a phase-change process with temperature-dependent thermal conductivity were obtained. Moreover, ten different cases were studied: four cases of free boundary problems (i.e. Stefan-like problems) and six cases of moving boundary problems (i.e. inverse Stefan-like problems).
The goal of this paper is to obtain a numerical sensitivity analysis of the mentioned ten cases for the simultaneous determination of unknown thermal coefficients and to determine the coefficients which are more sensitive with respect to the given parameters. We show numerical result for the aluminum.

1. Introduction

Heat transfer problems with a phase-change such as melting and freezing have been studied in the last century due to their wide scientific and technological applications. A review of a long bibliography on moving and free boundary problems for phase-change materials (PCM) for the heat equation is shown in [16].

We consider the following solidification problem for a semi-infinite material with an over specified condition on the fixed face $x=0$ [1,3,4,7]:

$$\begin{cases} i)\ \rho c T_t(x,t) = (k(T)T_x(x,t))_x, \quad 0<x<s(t),\ t>0 \\ ii)\ T(0,t) = T_o < T_f \quad, \quad t>0 \\ iii)\ k(T_o)T_x(0,t) = \dfrac{q_o}{\sqrt{t}} \quad, \quad t>0 \quad, \quad q_o>0 \\ iv)\ T(s(t),t) = T_f \quad, \quad t>0 \\ v)\ k\left(T_f\right)T_x(s(t),t) = \rho h \dot{s}(t), \quad t>0 \end{cases} \tag{1}$$

where $T(x,t)$ is the temperature of the solid phase, $\rho>0$ is the density of mass, $h>0$ is the latent heat of fusion by unity of mass, $c>0$ is the specific heat, $x=s(t)$ is the phase-change interface, T_f is the phase-change temperature, T_o is the temperature at the fixed face $x=0$ and q_o is the coefficient that characterizes the heat flux at $x=0$ given by Eq. (1*iii*), which must be obtained experimentally through a phase-change process [2]. We suppose that the thermal conductivity has the following expression [5]:

$$k = k(T) = k_o\left[1 + \beta(T-T_o)/\left(T_f-T_o\right)\right], \quad \beta\in\mathbb{R}. \tag{2}$$

Let $\alpha_o = k_o/\rho c$ be the coefficient of the diffusivity at the temperature T_o. We observe that if $\beta=0$, the problem (1) becomes the classical one-phase Lamé-Clapeyron-Stefan problem with an overspecified condition at the fixed face $x=0$, and for this problem the corresponding simultaneous determination of thermal coefficients was studied in [13,14]. The phase-change process with temperature-dependent thermal coefficient of the type (2) was firstly studied in [5]. Other papers related to determination of thermal coefficients are [8,10,11,17–20].

The solution to problem (1) is given by [5,15]:

$$\begin{cases} i)\ T(x,t) = T_o + \dfrac{\left(T_f-T_o\right)}{\Phi(\lambda)}\Phi(\eta), \quad \eta = \dfrac{x}{2\sqrt{\alpha_o t}} \quad, \quad 0<\eta<\lambda \\ ii)\ s(t) = 2\lambda\sqrt{\alpha_o t} \end{cases} \tag{3}$$

where $\Phi=\Phi(x)=\Phi_\delta(x)$ is the modified error function, for a given $\delta>-1$, the unique solution to the following boundary value problem in variable x, i.e:

$$\begin{cases} i)\ [(1+\delta\ \Phi'(x))\Phi'(x)]' + 2x\Phi'(x) = 0 \quad, \quad x>0, \\ ii)\ \Phi(0^+) = 0 \quad, \quad \Phi(+\infty) = 1 \end{cases} \tag{4}$$

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Nomenclature

c	Specific heat, J/ (kg°C)
h	Latent heat of fusion by unit of mass, J/kg
k	Thermal conductivity, W/(m°C)
q_o	Coefficient that characterizes the heat flux at $x=0$, kg/$s^{5/2}$
s	Position of the free or moving front, m
Ste	The Stefan number defined by Eq. (9), dimensionless
t	Time, s
T	Temperature, °C
x	Spatial coordinate, m

Greek symbols

α	Diffusivity coefficient, m^2/s
β	Coefficient that characterizes the thermal conductivity in Eq. (2), dimensionless
δ	Coefficient that characterizes the differential Eq. (4*i*), dimensionless
η	Similarity variable defined by Eq. (3), dimensionless
λ	Coefficient that characterizes the free boundary in Eq. (3*ii*), dimensionless
ρ	Density, kg/m^3
σ	Coefficient that characterizes the moving boundary in Eq. (3*ii*bis), $m/s^{1/2}$

Subscripts

f	Fusion
o	Initial in time or in space

and the unknown thermal coefficients must satisfy the following system of equations [15]:

$$\beta - \delta\ \Phi(\lambda) = 0 \tag{5}$$

$$[1+\delta\ \Phi(\lambda)]\frac{\Phi'(\lambda)}{\lambda\ \Phi(\lambda)} - \frac{2h}{c\left(T_f - T_o\right)} = 0 \tag{6}$$

$$\frac{\Phi'(0)}{\Phi(\lambda)} - \frac{2q_o}{\left(T_f - T_o\right)\sqrt{k_o \rho c}} = 0. \tag{7}$$

For the particular case $\delta=0$ we have that $\Phi(x)=erf(x)$ is the error function, which is defined by:

$$erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}\,du. \tag{8}$$

We remark that if problem (1) is a free boundary problem (this case can be considered as a Stefan problem) with an overspecified condition on the fixed face $x=0$, then the coefficient $\lambda>0$ is an unknown coefficient. On the other hand, if problem (1) is a moving boundary problem (this case can be considered as an inverse Stefan problem) with an overspecified condition on the fixed face $x=0$, then the phase-change interface will be given by

$$s(t) = 2\sigma\sqrt{t} \tag{3iibis}$$

where σ must be obtained experimentally ($\sigma = \lambda\sqrt{\alpha_o}$) through a phase-change process [2,14].

When the coefficient $\delta=0$, the corresponding determination of formulas for one or two unknown thermal coefficients were obtained in [13,14] and the numerical-experimental determination was given in [2]. When the coefficient $\delta\neq 0$ is given, the corresponding problem was analyzed in [15]; in this case, the necessary and sufficient conditions on the data were obtained in order to ensure the existence of the solution.

The goal of the present paper is to make the sensitivity analysis of the free and moving boundary problems, analyzed in [15]. For a one-phase Stefan problem, the temperature $T(x,t)$, the free boundary interface $s(t)$ (i.e. the coefficient λ, defined in Eq. (3*ii*), is also an unknown coefficient) and the following parameters in four different cases:

FB:	i) λ, β, k_o	ii) λ, β, ρ	iii) λ, β, h	iv) λ, β, c,

were determined in [15]. For a one-phase inverse Stefan problem (i.e. the interface $s(t)$ is given by Eq. (3*ii*bis) for a given $\sigma>0$), the temperature $T(x,t)$ and the following parameters in six cases:

MB:	i) β, k_o, ρ	ii) β, k_o, c	iii) β, k_o, h	iv) β, ρ, c	v) β, ρ, h	vi) β, c, h,

were also determined in [15].

The explicit formulas corresponding to the ten cases for the unknown thermal coefficients were summarized in [15] (see Table 1). For cases FB (iii and iv) and MB (ii, iv, v and vi) the data must satisfy certain restrictions in order to obtain the solution of the corresponding thermal problem. These restrictions, called R_1, R_2, R_3 and R_4 in [15], are the following:

$$\frac{\left(T_f - T_o\right)\Phi'(0)}{2q_o}\sqrt{k_o \rho c} < 1 \tag{R1}$$

$$\frac{\left(T_f - T_o\right)k_o \rho h}{2q_o^2} < 1 \tag{R2}$$

$$\frac{\rho\sigma h}{q_o} < 1 \tag{R3}$$

Table 1
Left and right normalized sensitivities in the four cases of free boundary problems.

Case number	Unknown Coefficients	δ		k_o		ρ		c		h	
1	λ	0.008	0.008	–	–	0	0	0.48	0.48	−0.48	−0.48
	β	1.01	1.01	–	–	0	0	0.46	0.46	−0.46	−0.46
	k_o	−0.015	−0.015	–	–	−1.01	−0.99	−0.082	−0.081	−0.92	−0.9
2	λ	0.008	0.008	0	0	–	–	0.48	0.48	−0.48	−0.48
	β	1.01	1.01	0	0	–	–	0.46	0.45	−0.46	−0.45
	ρ	−0.015	−0.015	−1.01	−0.99	–	–	−0.082	−0.081	−0.92	−0.9
3	λ	0.016	0.016	0.52	0.52	0.52	0.52	–	–	0.52	0.52
	β	1.02	1.02	0.5	0.49	0.5	0.49	–	–	0.5	0.49
	h	−0.016	−0.016	−1.1	−1.07	−1.1	−1.07	–	–	−0.089	−0.088
4	λ	−0.084	−0.084	−5.85	−6.08	−5.85	−6.08	−5.85	−6.08	–	–
	β	0.92	0.92	−5.52	−5.78	−5.52	−5.78	−5.52	−5.78	–	–
	c	−0.19	−0.19	−12.4	−12.1	−12.4	−12.1	−11.3	−11.2	–	–

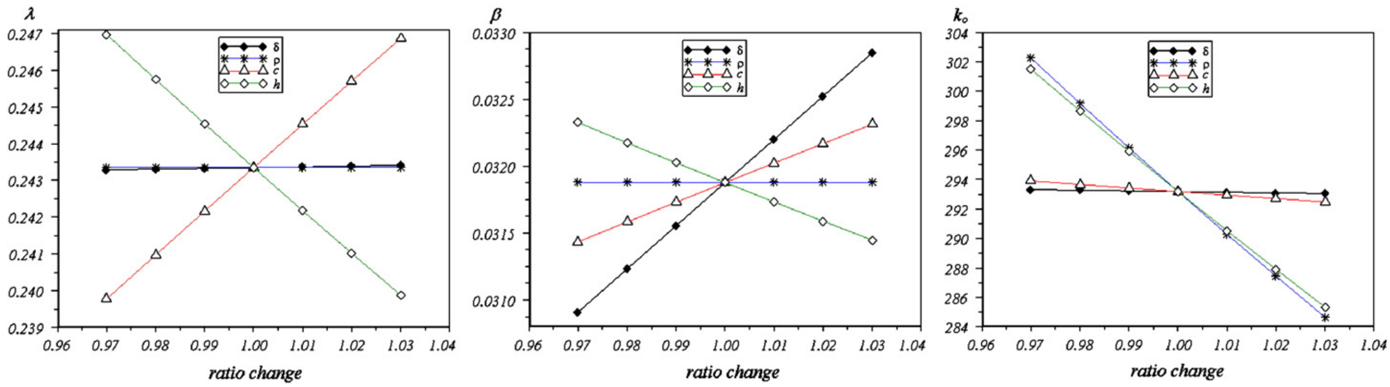

Fig. 1. Parametric change of {λ, β, k_o} versus the relative change of {δ, ρ, c, h} in Case 1 of the free boundary problem.

$$\frac{\left(T_f - T_o\right)k_o}{2\sigma q_o} < 1. \tag{R4}$$

2. Sensitivity analysis

We use the free software SCILAB for the numerical analysis. For each case, first we have to determine the solution to the corresponding system of equations. We use the command bvodeS to solve the differential problem (4), which allows us to evaluate the modified error function at the necessary points for a given $\delta > -1$. To find the solution to the different equations we minimize the absolute value, using the Levenberg-Marquardt algorithm. Secondly, using the approximately solution, we evaluate the unknown thermal coefficients.

In each case, we use the corresponding data, from the following set of values that satisfy Eq. (5)–(7). The data corresponding to aluminum near its melting point are:

$\beta = 0.0318778$	$\delta = 0.1177546$	$\lambda = 0.2433491$	$k_o = 293{,}1882$ W/m °C
$c = 783.6192$ J/kg °C	$\rho = 2698.4$ kg/m^3	$h = 388000$ J/kg	$q_o = 3179226.8$ kg/s$^{5/2}$
$T_f = 660$ °C	$T_o = 600$ °C	$\sigma = 0.0028655$ m/s$^{1/2}$	

In order to determine the influence of known parameters over unknown coefficients, we define the *normalized sensitivity* by the following expression [12]:

$$S(p, q_i) = \frac{q_i}{p}\left[\frac{\partial p}{\partial q_i}\right] \tag{9}$$

where p is a particular solution parameter (e.g., the dimensionless parameters β or λ, or the initial thermal conductivity k_o in Case 1 of the free boundary problems), q_i is one of the given parameters (e.g, δ, ρ, c, h in Case 1). Thanks to its dimensionless nature, we can compare the sensitivity of parameters of different magnitude. The normalized sensitivity indicates the percentage change on the value of the parameter p, when the variable q_i increases or decreases 1% of its value [6,9]. We will approximate $S(p,q_i)$ by the following way:

$$\begin{aligned} S(p,q_i)^+ &\approx \frac{q_i}{p(q)} \cdot \frac{p\left(\hat{q}^+\right) - p(q)}{\hat{q}_i^+ - q_i} \quad \text{right normalized sensitivity} \\ S(p,q_i)^- &\approx \frac{q_i}{p(q)} \cdot \frac{p\left(\hat{q}^-\right) - p(q)}{\hat{q}_i^- - q_i} \quad \text{left normalized sensitivity} \end{aligned} \tag{10}$$

where q is the vector $(q_1, \ldots\ldots q_i, \ldots\ldots)$, $p(q) = p(q_1, \ldots\ldots q_i, \ldots\ldots)$ and

$$\begin{aligned} \hat{q}_j^+ &= q_j, j \neq i \text{ and } \hat{q}_i^+ = q_i + \varepsilon|q_i| \\ \hat{q}_j^- &= q_j, j \neq i \text{ and } \hat{q}_i^- = q_i - \varepsilon|q_i| \end{aligned} \tag{11}$$

and $\varepsilon = 0.01$. Here the right normalized sensitivity represents the change on the parameter p when q_i increases a 1% of its value, and the left normalized sensitivity represents the change on the parameter p when q_i decreases 1%.

2.1. Determination of coefficients through a free boundary problem

We have analyzed the relationship between the solution of each case and the different parameters. Table 1 shows the right and the left normalized sensitivities, in each case, taking $\varepsilon = 0.01$. If the sensitivity

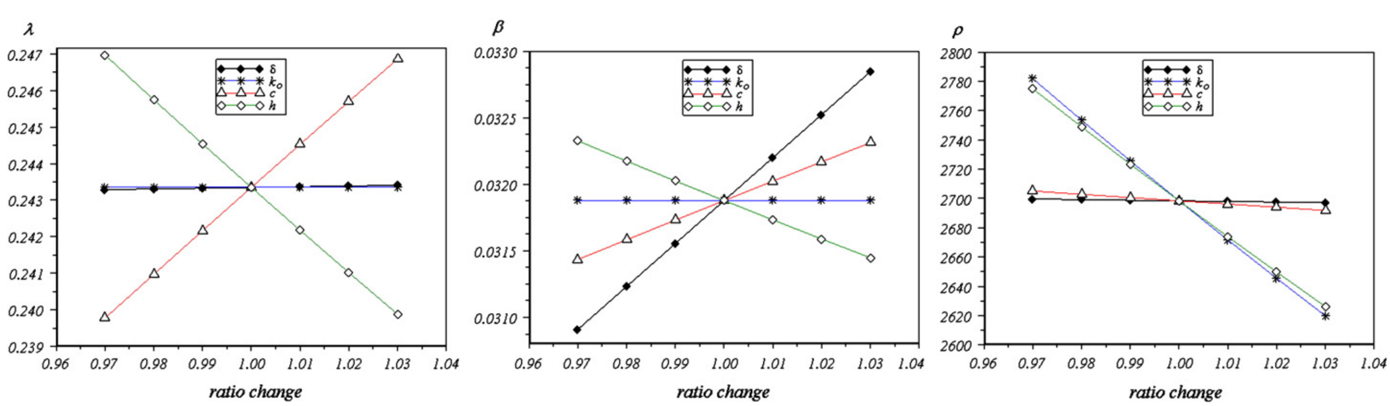

Fig. 2. Parametric change of {β, λ, ρ} versus the relative change of {δ, k_o, c, h} in Case 2 of the free boundary problem.

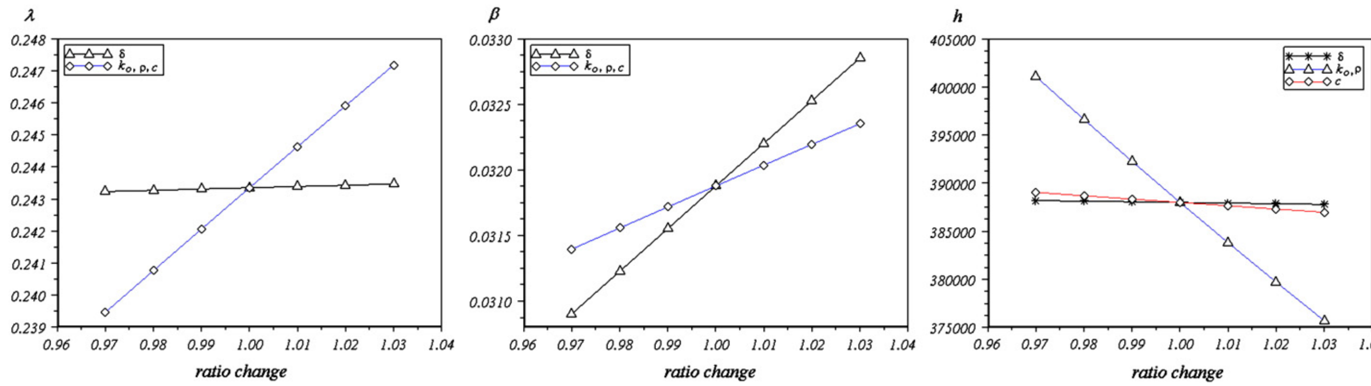

Fig. 3. Parametric change of {λ, β, h} versus the relative change of {δ, k_o, ρ, c} in Case 3 of the free boundary problem.

is negative, it means that the parameter p is decreasing with respect to q_i, and if it is positive, it means that the parameter p is increasing with respect to q_i.

2.1.1. Case 1 and 2

These two cases are analyzed together, because when we modify the parameters δ, c or h, the corresponding λ and β are the same for both cases. This can be explained observing that the equations to be solved for λ and β are the same in both cases. Another remark is that the parameters k_o or ρ do not appear explicitly in the equation for λ or β, therefore, these parameters remain constant when we modify the values of k_o or ρ. Figs. 1 and 2 show the relationship between the parameter solutions and the given parameters {δ, k_o, ρ, c and h} in Cases 1 and 2, respectively. The parameter λ is more sensitive to changes in h, the parameter β is more sensitive to changes in δ, and the parameters k_o and ρ are more sensitive to changes in ρ and k_o , respectively.

2.1.2. Case 3

We can observe that the parameters λ and β behave in the same way when we modify k_o, ρ or c. Fig. 3 shows the relationship between the parameter solutions {λ, β, h} and the given parameters {δ, k_o , ρ and c}. The parameter λ is more sensitive to changes in k_o , ρ and c, the parameter β is more sensitive to changes in δ, and h is more sensitive to changes in ρ and k_o .

2.1.3. Case 4

We can observe that the parameters λ and β behave in the same way when we modify k_o, ρ or h. Fig. 4 shows the relationship between the parameter solutions {λ, β, c} and the given parameters {δ, k_o, ρ and h}. The parameters λ and β are more sensitive to changes in k_o, ρ and h; and the parameter c is more sensitive to changes in ρ and k_o. The restriction R_2 was satisfied up to a 9.75% increase in the parameters k_o , ρ or h.

2.2. Determination of coefficients through a moving boundary problem

We have analyzed the relationship between the solution of each case and the different parameters. Table 2 shows the right and left normalized sensitivities, in each case, taking $\varepsilon = 0.01$.

2.2.1. Case 1

In this case, we can observe that the parameters λ, β and k_o behave in the opposite way when we modify c or h. Another remark is that in the equations for λ and β there is no intervention of σ, therefore these parameters remain constant when we modify the values of σ. Fig. 5 shows the relationship between the parameter solutions {β, k_o and ρ} and the given parameters {δ, σ, c and h}. The parameter β is more sensitive to changes in δ; the parameter k_o is more sensitive to changes in σ; and the parameter ρ is more sensitive to changes in σ and h.

2.2.2. Case 2

In this case, we can observe that the parameters λ and β behave in the same way when we modify σ, ρ or h. Instead, the parameter c behaves in the same way when we modify σ or ρ (but not h). On the other hand, the parameter k_o behaves in the same way when we modify h or ρ (but not σ). Fig. 6 shows the relationship between the parameter solutions {β, k_o, c} and the given parameters {δ, σ, ρ, h}. The parameter β is more sensitive to changes in σ, ρ and h; the parameter k_o is more sensitive to changes in σ; and the parameter c is more sensitive to changes in σ and ρ. The restriction R_3 was satisfied up to a 5.97% increase in the parameters σ, ρ or h.

2.2.3. Case 3

We can observe that the parameters λ and β behave in the same way when we modify σ, c or ρ. Instead, the parameter k_o behaves in the same way when we modify c or ρ (but not σ). On the other hand, the parameter h behaves in the same way when we modify σ or ρ (but

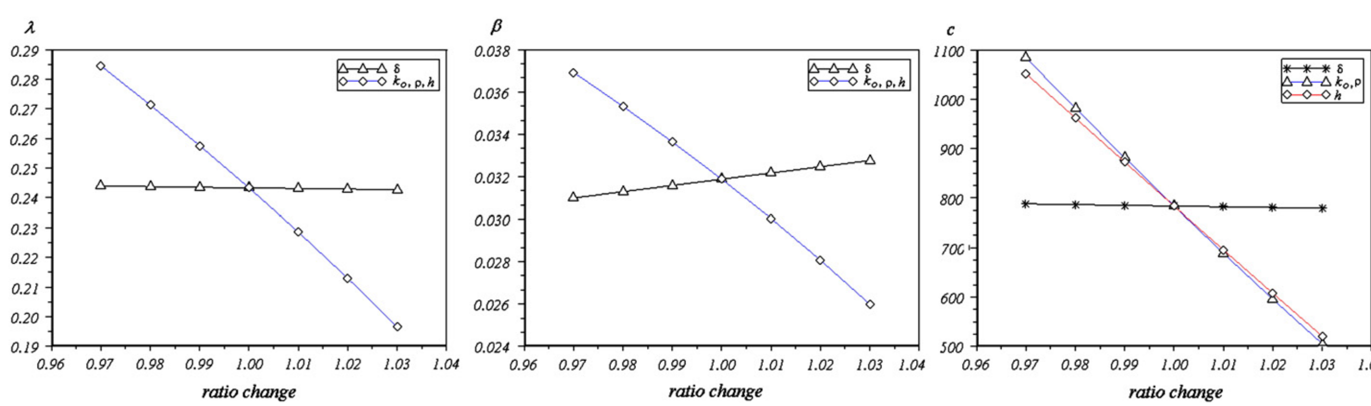

Fig. 4. Parametric change of {λ, β, c} versus the relative change of {δ, k_o, ρ, h} in Case 4 of the free boundary problem.

Table 2
Left and right normalized sensitivities in the six cases of moving boundary problems.

Case N°	Unknown Coeff.	δ		σ		k_o		ρ		c		H	
1	β	1.01	1.01	0	0	–	–	–	–	0.46	0.45	−0.46	−0.45
	k_o	−0.015	−0.015	1	1	–	–	–	–	−0.026	−0.025	0.025	0.025
	ρ	$2.9*10^{-4}$	$2.9*10^{-4}$	−1.01	−0.99	–	–	–	–	−0.056	−0.055	−0.95	−0.93
2	β	1.01	1.01	−7.92	−8.63	–	–	−7.92	−8.63	–	–	−7.92	−8.63
	k_o	−0.016	−0.016	1.45	1.47	—	—	0.45	0.46	—	—	0.45	0.46
	c	0.0052	0.0052	−18.1	−17.7	–	–	−18.1	−17.7	–	–	−17	−16.9
3	β	1.01	1.01	0.48	0.48	–	–	0.48	0.48	0.48	0.48	–	–
	k_o	−0.015	−0.015	0.97	0.97	–	–	−0.027	−0.027	−0.027	−0.027	–	–
	h	$3.1*10^{-4}$	$3.1*10^{-4}$	−1.07	−1.04	–	–	−1.07	−1.04	−0.059	−0.059	–	–
4	β	0.73	0.72	19.5	16.6	−16.8	−19.3	–	–	–	–	0	0
	ρ	0.034	0.034	−3.15	−3.16	2.22	2.1	–	–	–	–	−1	−0.99
	c	−0.61	−0.6	37.2	40.5	−41	−36.9	–	–	–	–	0.99	1
5	β	0.73	0.72	19.5	16.6	−16.8	−19.3	–	–	0	0	–	–
	ρ	−0.58	−0.57	35.2	36.1	−37.8	−35.5	–	–	−1	−0.99	–	–
	h	0.61	0.61	−59.4	−28.8	29.1	58.5	–	–	1	1	–	–
6	β	0.73	0.72	19.5	16.6	−16.8	−19.3	0	0	–	–	–	–
	c	−0.58	−0.57	35.2	36.1	−37.8	−35.5	−1	−0.99	–	–	–	–
	h	0.034	0.034	−3.15	−3.16	2.22	2.1	−1	−0.99	–	–	–	–

not c). Fig. 7 shows the relationship between the parameter solutions $\{\beta, k_o$ and $h\}$ and the given parameters $\{\delta, \sigma, \rho$ and $c\}$. The parameter β is more sensitive to changes in δ; the parameter k_o is more sensitive to changes in σ; and the parameter h is more sensitive to changes in ρ and σ. The restriction R_4 was satisfied up to a 3.57% increase in the initial thermal conductivity k_o, and up to a 3.45% decrease in the parameter σ.

2.2.4. Case 4, 5 and 6

In all these three cases, the equations for the parameters λ and β are the same. The only three parameters that appear at these equations are δ, σ and k_o; neither h, c or ρ are involved in the equation for λ or β. This means that λ and β maintain constant when we modify c (in Case 4), h (in Case 5) or ρ (in Case 6). Figs. 8–10 show the relationship between the parameter solutions and the other given parameters, in Cases 4, 5 and 6, respectively. The parameter β is more sensitive to changes in σ and k_o; and the most influential parameters are σ and k_o, for the rest of the given parameters.

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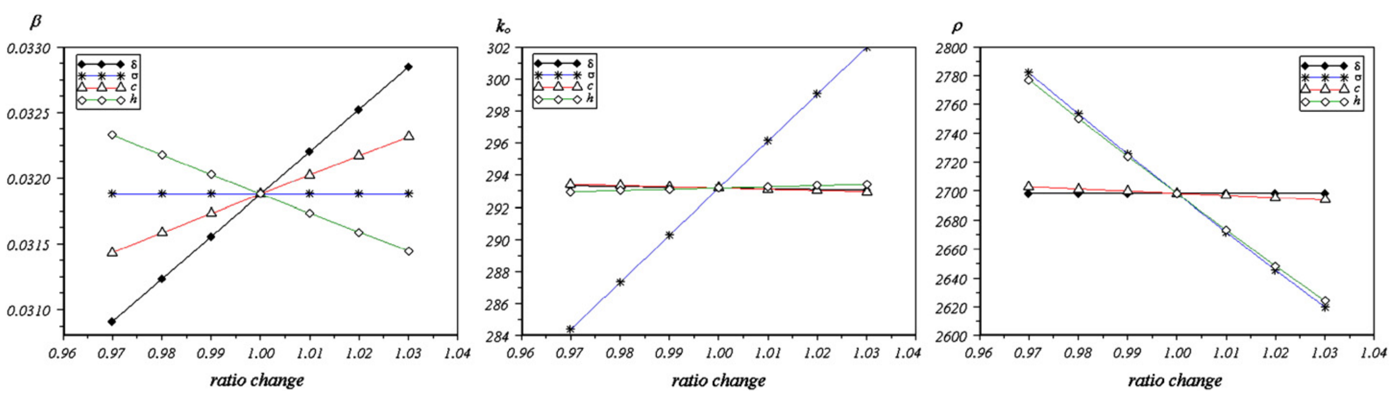

Fig. 5. Parametric change of $\{\beta, k_o, \rho\}$ versus the relative change of $\{\delta, \sigma, c, h\}$ in Case 1 of the moving boundary problem.

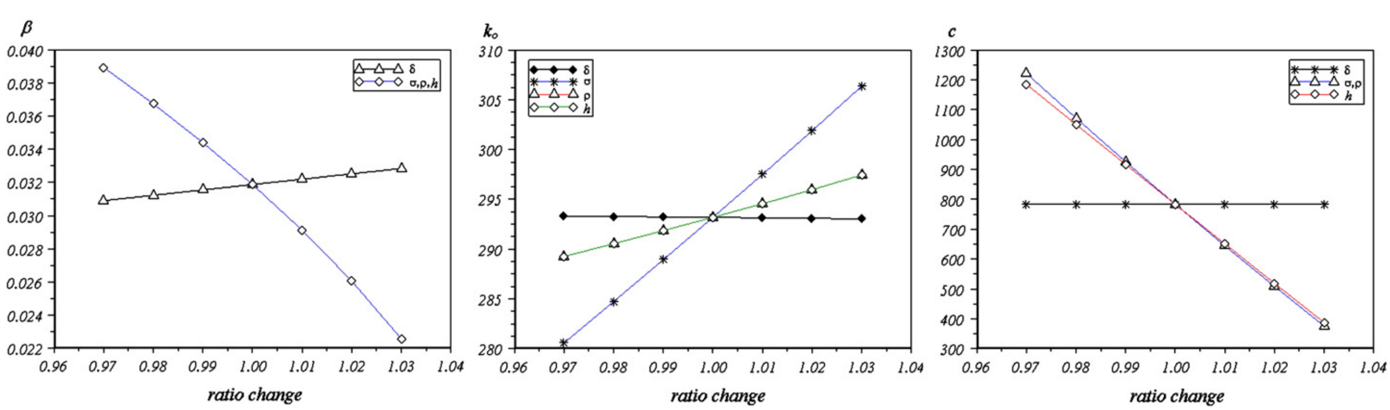

Fig. 6. Parametric change of $\{\beta, k_o, c\}$ versus the relative change of $\{\delta, \sigma, \rho, h\}$ in Case 2 of the moving boundary problem.

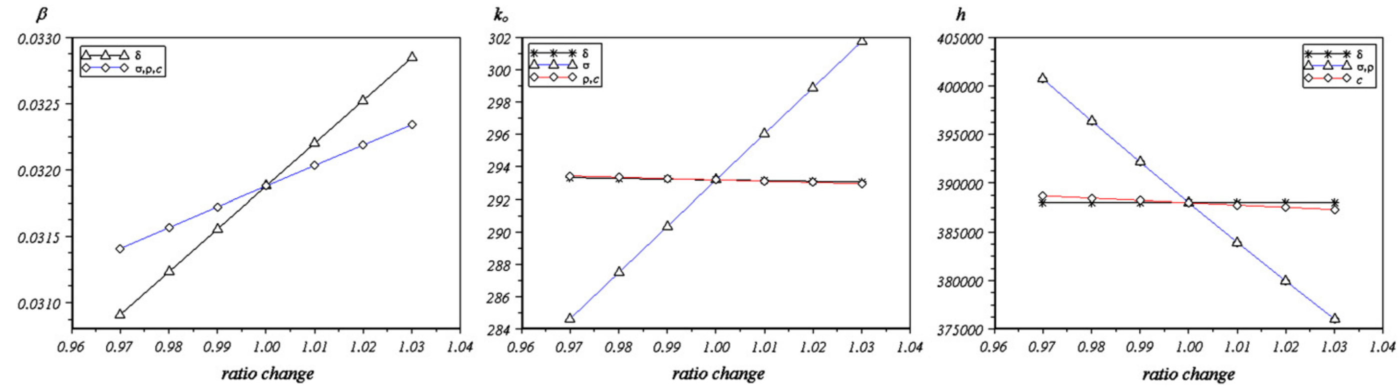

Fig. 7. Parametric change of {β, k_o, h} versus the relative change of {δ, σ, ρ, c} in Case 3 of the moving boundary problem.

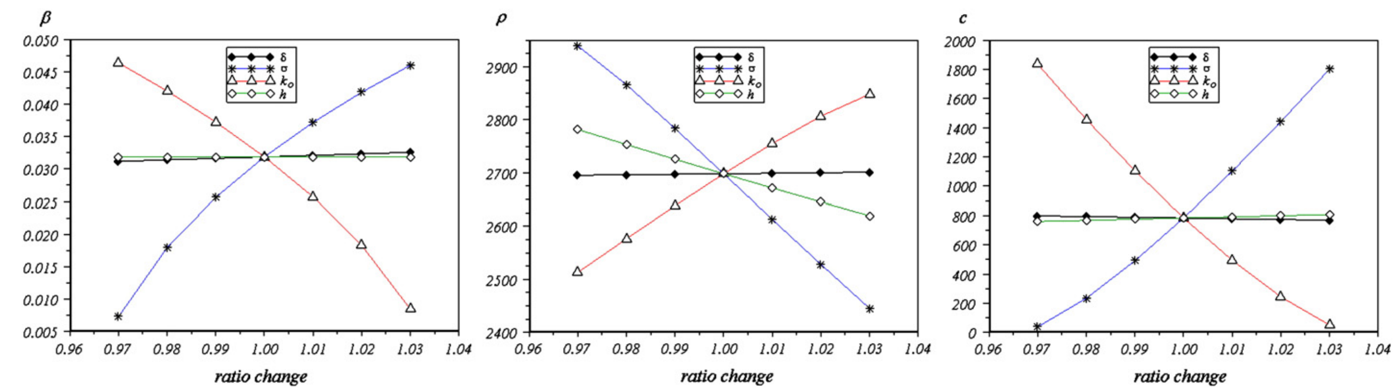

Fig. 8. Parametric change of {β, ρ, c} versus the relative change of {δ, σ, k_o, h} in Case 4 of the moving boundary problem.

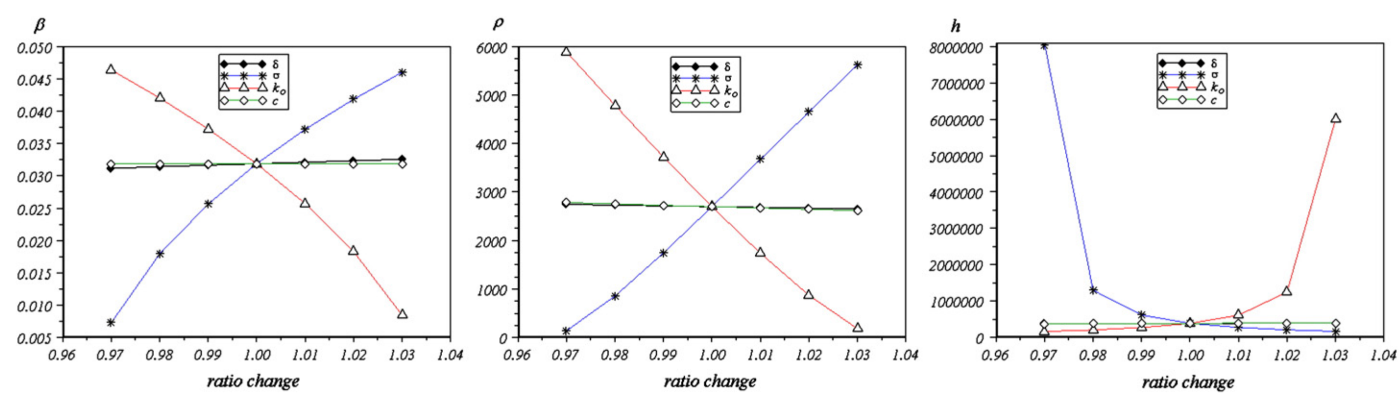

Fig. 9. Parametric change of {β, ρ, h} versus the relative change of {δ, σ, k_o, c} in Case 5 of the moving boundary problem.

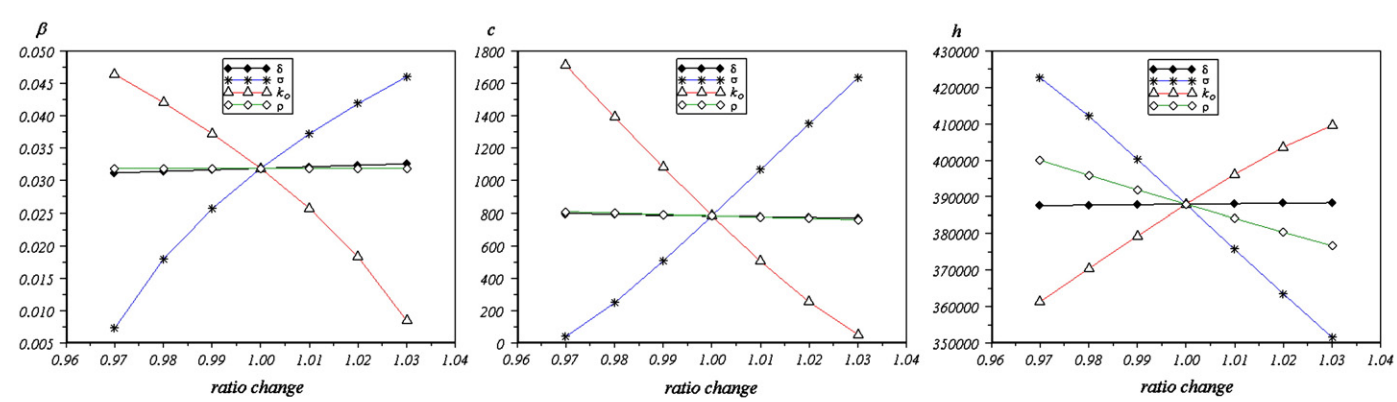

Fig. 10. Parametric change of {β, c, h} versus the relative change of {δ, σ, k_o, ρ} in Case 6 of the moving boundary problem.

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