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NUMERICAL ANALYSIS FOR THE HEAT FLUX IN A MIXED ELLIPTIC PROBLEM TO OBTAIN A DISCRETE STEADY-STATE TWO-PHASE STEFAN PROBLEM*

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Abstract. We consider a material $\Omega \subset \mathbb{R}^n$ which occupies a convex polygonal bounded domain with regular boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ (with $\overset{\circ}{\Gamma}_1 \cap \overset{\circ}{\Gamma}_2 = \emptyset$) with meas$(\Gamma_1) = |\Gamma_1| > 0$ and $|\Gamma_2| > 0$. We assume, without loss of generality, that the melting temperature is 0°C. We apply a temperature $b = \text{Const} > 0$ on Γ_1 and a heat flux $q = \text{Const} > 0$ on Γ_2. We consider a steady-state heat conduction problem in Ω.

We consider a regular triangulation of the domain Ω with Lagrange triangles of type 1. We study sufficient (and/or necessary) conditions on the heat flux q on Γ_2 to obtain a change of phase (steady-state, two-phase, discretized Stefan problem) in the corresponding discretized domain, that is, a discrete temperature of nonconstant sign in Ω.

Key words. steady-state Stefan problem, finite element method, mixed elliptic problem, numerical analysis, variational inequalities, error bounds

AMS subject classifications. 35R35, 35J85, 65N15, 65N30

1. Introduction. We consider a material $\Omega \subset \mathbb{R}^n$ which occupies a convex polygonal bounded domain with a regular boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ (with $\overset{\circ}{\Gamma}_1 \cap \overset{\circ}{\Gamma}_2 = \emptyset$) with meas $(\Gamma_1) = |\Gamma_1| > 0$ and $|\Gamma_2| > 0$. We assume, without loss of generality, that the melting temperature is 0°C. We apply a temperature $b = \text{Const} > 0$ on Γ_1 and a heat flux $q = \text{Const} > 0$ on Γ_2. We consider a steady-state heat conduction problem in Ω. Following [10], we study the temperature $\theta = \theta(x)$ for $x \in \Omega$. The set Ω can be written by

$$\Omega = \Omega_1 \cup \Omega_2 \cup \mathcal{L}, \tag{1}$$

where

$$\begin{aligned} \Omega_1 &= \{x \in \Omega / \theta(x) < 0\} \ \text{(solid phase)}, \\ \Omega_2 &= \{x \in \Omega / \theta(x) > 0\} \ \text{(liquid phase)}, \\ \mathcal{L} &= \{x \in \Omega / \theta(x) = 0\} \ \text{(free boundary)}, \end{aligned} \tag{2}$$

are, respectively, the solid phase, the liquid phase, and the free boundary which separates them. The temperature θ can be represented in Ω in the following way:

$$\theta(x) = \begin{cases} \theta_1(x) < 0, & x \in \Omega_1, \\ 0, & x \in \mathcal{L}, \\ \theta_2(x) > 0, & x \in \Omega_2, \end{cases} \tag{3}$$

and satisfies the conditions

$$\begin{aligned} &\Delta\theta_i = 0 \quad \text{in } \Omega_i \ (i = 1, 2), \\ &\theta_1 = \theta_2 = 0, \quad k_1 \frac{\partial \theta_1}{\partial n} = k_2 \frac{\partial \theta_2}{\partial n} \quad \text{on } \mathcal{L}, \\ &\theta_2|_{\Gamma_1} = b > 0, \\ &-k_2 \frac{\partial \theta_2}{\partial n}\Big|_{\Gamma_2} = q \quad \text{if } \theta|_{\Gamma_2} > 0, \\ &-k_1 \frac{\partial \theta_1}{\partial n}\Big|_{\Gamma_2} = q \quad \text{if } \theta|_{\Gamma_2} < 0, \end{aligned} \tag{4}$$

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where $k_i > 0$ is the thermal conductivity in Ω_i ($i = 1$: solid phase, $i = 2$: liquid phase). If we introduce the new unknown function [3, 10]

$$u = k_2\theta^+ - k_1\theta^- \left(\theta = \frac{1}{k_2}u^+ - \frac{1}{k_1}u^-\right) \quad \text{in } \Omega, \tag{5}$$

where θ^+ and θ^- represent the positive part and the negative part of the function θ, respectively, then problem (4) is transformed into the mixed elliptic problem

$$\begin{aligned} &\Delta u = 0 \quad \text{in } \Omega, \\ &u|_{\Gamma_1} = B, \\ &-\frac{\partial u}{\partial n}|_{\Gamma_2} = q, \end{aligned} \tag{6}$$

whose variational formulation is given by

$$\begin{aligned} &a(u, v-u) = L(v-u) \quad \forall v \in K, \\ &u \in K, \end{aligned} \tag{7}$$

where

$$\begin{aligned} &V = H^1(\Omega), \quad B = k_2 b > 0 \quad \text{on } \Gamma_1, \\ &K = \left\{v \in V / v|_{\Gamma_1} = B\right\}, \quad V_o = \left\{v \in V / v|_{\Gamma_1} = 0\right\}, \\ &a(u, v) = \int_\Omega \nabla u . \nabla v \, dx, \quad L(v) = L_q(v) = -\int_{\Gamma_2} qv \, d\gamma. \end{aligned} \tag{8}$$

Moreover, the solution of (7) is characterized by the minimization problem [5]:

$$\begin{aligned} &J(u) \leq J(v) \quad \forall v \in K, \\ &u \in K, \end{aligned} \tag{9}$$

where

$$J(v) = J_q(v) = \frac{1}{2}a(v, v) - L_q(v) = \frac{1}{2}a(v, v) + \int_{\Gamma_2} qv \, d\gamma. \tag{10}$$

We can define the real function $f : \mathbb{R}^+ \to \mathbb{R}$ in the following way:

$$f(q) = J_q(u(q)) = \frac{1}{2}a(u(q), u(q)) + q\int_{\Gamma_2} u_q \, d\gamma, \tag{11}$$

where $u = u(q)$ is the unique solution of the variational equality (7) for each heat flux $q > 0$ (for a given $B > 0$).

The evolution of the Stefan problem with mixed boundary conditions is considered in [7, 8].

For the continuous problem (6) or (7), a sufficient condition to have a steady-state two-phase Stefan problem (i.e., the solution of $u(q)$ of (7) is a function of nonconstant sign in Ω) was obtained in [11, 12] in terms of qualitative properties of f.

THEOREM 1. (i) *The function f is differentiable. Moreover, f' is a continuous and strictly decreasing function and it is given by*

$$f'(q) = \int_{\Gamma_2} u(q) \, d\gamma. \tag{12}$$

(ii) *There exists a geometric constant* $C = C(\Omega, \Gamma_1, \Gamma_2) > 0$ *such that*

$$a(u(q), u(q)) = Cq^2, \quad f(q) = -\frac{C}{2}q^2 + B|\Gamma_2|q \quad \forall q > 0. \tag{13}$$

Moreover, the constant $C > 0$ *is given by*

$$C = a(u_3, u_3) = \int_{\Gamma_2} u_3\, d\gamma > 0, \tag{14}$$

where $u_3 \in V_o$ $(u(q) = B - qu_3$ *in* $\Omega)$ *is the unique solution of the mixed elliptic problem*

$$\begin{aligned} &\Delta u_3 = 0 \text{ in } \Omega, \\ &u_3|_{\Gamma_1} = 0, \quad \frac{\partial u_3}{\partial n}|_{\Gamma_2} = 1, \end{aligned} \tag{15}$$

whose variational formulation is given by

$$\begin{aligned} &a(u_3, v) = \int_{\Gamma_2} v\, d\gamma \quad \forall v \in V_o, \\ &u_3 \in V_o. \end{aligned} \tag{16}$$

(iii) *If*

$$q > q_0(B), \tag{17}$$

then (6) *or* (7) *represents a steady-state two-phase Stefan problem (i.e., the solution* $u(q)$ *of problem* (7) *is a function of nonconstant sign in* Ω*), where* $q_0 = q_0(B)$ *is given by*

$$q_0(B) = \frac{B|\Gamma_2|}{C} \quad \forall B > 0. \tag{18}$$

(iv) *If the function* $u(q)$ *is constant over* Γ_2*, then the sufficient condition (given by* (17)*) is also necessary.*

Proof. See [12].

Now, we consider τ_h, a regular triangulation of the polygonal domain Ω with Lagrange triangles of type 1, constituted by affine-equivalent finite element of class C°, where $h > 0$ is a parameter which goes to zero. We can take h equal to the longest side of the triangles $T \in \tau_h$ and we can approximate V_o by [2]:

$$V_h = \left\{ v_h \in C^0(\bar{\Omega}) / v_h|_T \in P_1(T), \forall T \in \tau_h, v_h|_{\Gamma_1} = 0 \right\}, \tag{19}$$

where P_1 is the set of the polynomials of degree less than or equal to 1. Let Π_h be the corresponding linear interpolation operator. Then there exists a constant $C_o > 0$ (independent of the parameter h) such that

$$\|v - \Pi_h v\|_V \le C_o h^{r-1} \|v\|_{r,\Omega}, \quad \forall v \in H^r(\Omega), \quad \text{with } 1 < r \le 2. \tag{20}$$

We consider the following finite-dimensional approximate variational problem, corresponding to the continuous variational problem (7), given by

$$\begin{aligned} &a(u_h, v_h) = L(v_h), \quad \forall v_h \in V_h, \\ &u_h \in K_h = B + V_h, \end{aligned} \tag{21}$$

and we can obtain the following results.

LEMMA 2. *We have*

(22) $$\lim_{h\to 0^+} \|u_h - u\|_V = 0,$$

where u is the unique solution of the variational equality (7).

Proof. Since meas$(\Gamma_1) > 0$, we have that the bilinear form a is coercive over V_o; that is [5],

(23) $$\exists \alpha > 0 / a(v, v) = \|v\|^2_{V_o} \geq \alpha \|v\|^2_V, \quad \forall v \in V_o,$$

and therefore $\|\cdot\|_{V_o}$ and $\|\cdot\|_V$ are two equivalent norms in V_o. We conclude the proof by following a method similar to the one developed in [2].

COROLLARY 3. *If we define*

(24) $$\theta_h = \frac{1}{k_2} u_h^+ - \frac{1}{k_1} u_h^- \in V, \quad \theta = \frac{1}{k_2} u^+ - \frac{1}{k_1} u^- \in V,$$

then we have

(25) $$\lim_{h\to 0^+} \|\theta_h - \theta\|_H = 0,$$

where $H = L^2(\Omega)$.

Proof. If we consider the scalar product in H, defined by

(26) $$(u, v) = \int_\Omega u\, v\, dx,$$

then we deduce

(27) $$\|u_h - u\|^2_H = \|u_h^+ - u^+\|^2_H + \|u_h^- - u^-\|^2_H + 2(u_h^+, u^-) + 2(u_h^+, u^+) \geq \|u_h^+ - u^+\|^2_H + \|u_h^- - u^-\|^2_H;$$

that is,

(28) $$\text{Max}(\|u_h^+ - u^+\|, \|u_h^- - u^-\|) \leq \|u_h - u\|_H.$$

From (24) we obtain

(29) $$\|\theta_h - \theta\|_H \leq \frac{1}{k_2}\|u_h^+ - u^+\|_H + \frac{1}{k_1}\|u_h^- - u^-\|_H \leq \left(\frac{1}{k_1} + \frac{1}{k_2}\right)\|u_h - u\|_H;$$

that is, (25) holds.

The goal of this paper is to consider the discrete equivalent of the inequality (17). We study sufficient (and/or necessary) conditions on the constant heat flux q on Γ_2 to obtain a change of phase (steady-state, two-phase, discretized Stefan problem) in the corresponding discretized domain, that is a discrete temperature of nonconstant sign in Ω. We obtain the following.

(i) There exists a constant $C_h > 0$ (which depends only on the geometry of the domain Ω for each $h > 0$ and which is characterized by a variational problem) such that if $q > q_{0_h}(B) = B|\Gamma_2|/C_h$ then the steady-state discretized problem presents two phases.

(ii) We have the estimations $C_h < C$ and $q_0(B) < q_{0_h}(B)$, where C and $q_0(B)$ are given for the continuous problem by (14) and (18), respectively, (see [12]).

(iii) We deduce an error bound for $C - C_h$ and $q_{0_h}(B) - q_0(B)$ as a function of the parameter h.

In other words, we obtain for the mixed elliptic discretized problem, defined by u_h, analogous conditions to the ones obtained for the corresponding continuous problem [12] defined by u.

2. Inequality for the heat flux in the discretized problem. For each $q > 0$ we consider the functions $u(q) \in K$ and $u_h(q) \in K_h$, respectively, as the unique solution of the variational equalities (7) (continuous problem) and (21) (discrete problem). For each $h > 0$, we define the real function $f_h : \mathbb{R}^+ \to \mathbb{R}$ in the following way:

$$f_h(q) = J_q(u_h(q)) = \frac{1}{2}a(u_h(q), u_h(q)) + q \int_{\Gamma_2} u_h(q)\, d\gamma, \quad q > 0. \tag{30}$$

We obtain the following properties.

THEOREM 4. (i) *If $u_i = u_h(q_i)$ is the solution of* (21) *for $q_i > 0$ $(i = 1, 2)$, then we have the relations*

$$a(u_2 - u_1, u_2 - u_1) = (q_1 - q_2) \int_{\Gamma_2} (u_2 - u_1)\, d\gamma, \tag{31}$$

$$a(u_2, u_2) - a(u_1, u_1) = a(u_2 + u_1, u_2 - u_1) = (q_1 + q_2) \int_{\Gamma_2} (u_1 - u_2)\, d\gamma. \tag{32}$$

(ii) *For all real numbers $q > 0$ and δ such that $(q + \delta) > 0$, we obtain the estimations*

$$\left\| \frac{1}{\delta}[u_h(q) - u_h(q+\delta)] \right\|_V \le D_1 = \frac{\|\gamma_o\|}{\alpha} |\Gamma_2|^{\frac{1}{2}}, \tag{33}$$

$$\left\| \frac{1}{\delta}[u_h(q) - u_h(q+\delta)] \right\|_{L^2(\Gamma_2)} \le D_2 = D_1 \|\gamma_o\|, \tag{34}$$

where γ_o is the linear and continuous trace operator defined over V and α is given by (23). *Moreover, the function $\mathbb{R}^+ \to \mathbb{R}$,*

$$q \to \int_{\Gamma_2} u_h(q)\, d\gamma \in \mathbb{R}, \tag{35}$$

is a continuous and strictly decreasing function.

(iii) *The function $f_h = f_h(q)$ is differentiable. Moreover, f_h' is a continuous and strictly decreasing function given by*

$$f_h'(q) = \int_{\Gamma_2} u_h(q)\, d\gamma. \tag{36}$$

Proof. (i) If we take $v = u_2 - u_1 \in V_h$ in the variational equality corresponding to u_1 and $v = u_1 - u_2 \in V_h$ in the one corresponding to u_2 and add and subtract the resulting relations, then we obtain (31) and (32), respectively.

(ii) Taking into account (23), the Cauchy–Schwarz inequality, and the continuity of the operator γ_o, we deduce (33). From (33) and the continuity of γ_o we have (34). Therefore, we have (35) because

$$\left| \int_{\Gamma_2} [u_h(q) - u_h(q+\delta)]\, d\gamma \right| \le D_2 |\Gamma_2|^{\frac{1}{2}} \delta. \tag{37}$$

Moreover, the monotony property is a consequence of (31).

(iii) From (30) and elementary computations, we deduce

$$\frac{1}{\delta}[f_h(q+\delta) - f_h(q)] = \frac{1}{2} \int_{\Gamma_2} [u_h(q) + u_h(q+\delta)]\, d\gamma, \tag{38}$$

that is (36), by using (35).

THEOREM 5. (i) *The element* $u_h = u_h(q) \in V_h$ *can be written as*

$$u_h(q) = B - q u_{3h} \tag{39}$$

where u_{3h} *is the unique solution of the variational equality*

$$\begin{aligned} & a(u_{3h}, v_h) = \int_{\Gamma_2} v_h \, d\gamma \quad \forall v_h \in V_h, \\ & u_{3h} \in V_h. \end{aligned} \tag{40}$$

(ii) *There exists a constant* $C_h > 0$ *such that*

$$f_h(q) = q\, B|\Gamma_2| - \frac{1}{2} C_h q^2 \quad \forall q > 0, \tag{41}$$

$$a(u_h(q), u_h(q)) = C_h q^2 \quad \forall q > 0, \tag{42}$$

where the constant C_h *is given by*

$$C_h = a(u_{3_h}, u_{3_h}) = \int_{\Gamma_2} u_{3_h} \, d\gamma. \tag{43}$$

(iii) *If* $q > q_{0_h}(B)$, *then problem* (21) *represents a discretized steady-state two-phase Stefan problem (i.e.,* $u_h(q)$ *is a function of a nonconstant sign in* Ω*), where*

$$q_{0_h}(B) = \frac{B|\Gamma_2|}{C_h}. \tag{44}$$

Proof. (i) follows from (21), (30), and (39) by uniqueness of the variational equalities (21) and (40).

(ii) follows from (8), (30), and (39).

(iii) follows taking into account

$$f_h'(q_{0_h}(B)) = 0 \tag{45}$$

and the monotony property of the function f_h'.

Remark 1. We have

$$u_h(0^+) = B, \quad f_h(0^+) = B|\Gamma_2|q, \quad f_h'(0^+) = B|\Gamma_2|. \tag{46}$$

THEOREM 6. (i) *We have the equality*

$$a(u(q), u_h(q)) = C_h q^2 \quad \forall q > 0. \tag{47}$$

(ii) *Also, we have the inequalities*

$$C_h < C, \tag{48a}$$

$$q_0(B) < q_{0_h}(B). \tag{48b}$$

Proof. (i) If we take $v = u_h(q) \in K_h = B + V_h \subset B + V_o = K$ in the variational equality (7), and we take into account the expressions (13) and (41), then we obtain (47).

(ii) On the other hand, from (23) and (47) we have

$$\alpha \|u(q) - u_h(q)\|_V^2 \le a(u(q) - u_h(q), u(q) - u_h(q)) = (C - C_h) q^2, \tag{49}$$

that is (48a). Moreover, (48b) follows from (18), (44), and (48a).

Now we shall use the interpolation result (20) for the function $u_3 \in H^r(\Omega)$ as a hypothesis of regularity of the continuous problem (7) (in general, $1 < r < 3/2$ [1, 4, 6, 9]). In [11] three examples with explicit solutions were presented. In those cases $u(q), u_3 \in C^\infty(\Omega)$.

THEOREM 7. *We have the relations and estimations*

$$a(u(q) - u_h(q), v_h) = 0 \quad \forall v_h \in V_h, \tag{50}$$

$$\begin{aligned}(C - C_h)q^2 &= a(u(q) - u_h(q), u(q) - u_h(q)) \\ &\leq \operatorname*{Inf}_{v_h \in V_h} a(u(q) - v_h, u(q) - v_h),\end{aligned} \tag{51}$$

$$0 < C - C_h \leq C_o^2 h^{2(r-1)} |u_3|^2_{r,\Omega}, \tag{52}$$

$$0 < q_{0_h}(B) - q_0(B) \leq \frac{C_o^2 h^{2(r-1)}}{C} |u_3|^2_{r,\Omega}\, q_{0_h}(B). \tag{53}$$

Proof. If we take $v = v_h \in V_h \subset V_o$ in the variational equality (7) and subtract from it with the variational equality (21), we obtain (50). By using (47), (49), and (50) we deduce

$$\begin{aligned}&a(u(q) - u_h(q), u(q) - u_h(q)) \\ &\quad = a(u(q) - u_h(q), u(q)) - a(u(q) - u_h(q), u_h(q)) \\ &\quad = a(u(q) - u_h(q), u(q)) - a(u(q) - u_h(q), v_h) \\ &\quad = a(u(q) - u_h(q), u(q) - v_h) \leq [a(u(q) - u_h(q), u(q) - u_h(q))]^{\frac{1}{2}} \\ &\qquad \cdot [a(u(q) - v_h, u(q) - v_h)]^{\frac{1}{2}} \quad \forall v_h \in V_h,\end{aligned} \tag{54}$$

because $a(.,.)$ is a scalar product in V_o; then we obtain (51).

By using (51), the facts that

$$\Pi_h(u(q)) \in B + V_h, \quad u(q) - \Pi_h(u(q)) \in V_h, \tag{55}$$

and the interpolation result (20), we deduce (52). The relation (53) is obtained by using the definitions of $q_{0_h}(B)$ and $q_0(B)$ and (52).

Remark 2. If we only have $u(q) \in V$ (i.e., $u_3 \in V$), we can obtain

$$0 < C - C_h \leq \frac{1}{q^2} \|u(q) - \Pi_h(u(q))\|_V^2 = \|u_3 - \Pi_h(u_3)\|_V^2, \tag{56}$$

where the second term converges to zero when $h \to 0^+$ [2], but we cannot give an order of convergence.

Remark 3. If the constant heat flux on Γ_2 verifies the inequality $q > q_{0_h}(B)$, then both the discrete and continuous problems represent steady-state two-phase Stefan problems; that is, their temperatures are of nonconstant sign in Ω.

Remark 4. When the function $u_h(q)$ is constant on Γ_2 (as a function of $x \in \Gamma_2$), then the sufficient condition given by Theorem 5(iii) is also necessary in order to have a two-phase discrete problem, because

$$\int_{\Gamma_2} u_h(q)\, d\gamma < 0 \Leftrightarrow u_h(q) < 0 \text{ on } \Gamma_2. \tag{57}$$

THEOREM 8. *If we let h, $B > 0$, and $0 < \epsilon_o < 1$ (ϵ_o is a parameter to be chosen arbitrarily), then we have the estimations*

$$q_o(B) < q_{o_h}(B) \leq \frac{q_o(B)}{\epsilon_o} \text{ and } C_h \geq C\,\epsilon_o, \quad \forall h \leq h_r(\epsilon_o), \tag{58}$$

$$0 < q_{o_h}(B) - q_o(B) \leq \frac{C_o^2 |u_3|_{r,\Omega}^2}{C\,\epsilon_o} q_o(B) h^{2(r-1)}, \quad \forall h \leq h_r(\epsilon_o), \tag{59}$$

where

$$h_r(\epsilon_o) = \left(\frac{C(1-\epsilon_o)}{C_o^2 |u_3|_{r,\Omega}^2} \right)^{\frac{1}{2(r-1)}}. \tag{60}$$

Proof. From (53) we deduce

$$A(h) q_{0_h}(B) \leq q_0(B), \tag{61}$$

where

$$A(h) = 1 - \frac{C_o^2 |u_3|_{r,\Omega}^2}{C} h^{2(r-1)} < 1. \tag{62}$$

If we consider, for each ϵ_0, $0 < \epsilon_o < 1$, the equivalence

$$0 < \epsilon_o < A(h) < 1 \Leftrightarrow 0 < h < h_r(\epsilon_o), \tag{63}$$

then we deduce the inequalities (58) and (59).

COROLLARY 9. *If $B > 0$, then we have the limit*

$$\lim_{h \to 0^+} q_{o_h}(B) = q_o(B). \tag{64}$$

Remark 5. If $r = 2$ then the convergence in Corollary 9 is of the order of h.

Remark 6. Everything we proved in this paper is still valid if the boundary Γ of the bounded domain Ω is represented by the union of three portions ($\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$) having the following characteristics:

(i) Γ_1 and Γ_2 have the same conditions as the ones previously described in (4).

(ii) Γ_3 is a wall impermeable to heat; i.e., we have $\frac{\partial\theta}{\partial n}|_{\Gamma_3} = 0$ in (4) and therefore $\frac{\partial u}{\partial n}|_{\Gamma_3} = 0$ in (6).

Moreover, the first example considered in [11] verifies this condition.

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