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CONVERGENCE OF A LATTICE NUMERICAL METHOD FOR A BOUNDARY-VALUE PROBLEM WITH FREE BOUNDARY AND NONLINEAR NEUMANN BOUNDARY CONDITIONS*

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Abstract. We consider the Stefan-type diffusion boundary-value problem with free boundary and nonlinear Neumann boundary conditions. Such problems describe hydride formation under constant conditions when nonlinear surface processes are taken into account. We construct the difference numerical method and prove the convergence of the interpolation approximations to the weak solution of the problem. Then we apply the theory of boundary-value problems to show that this weak solution is the classical solution. Thus, the existence of the solution to the problem is proved and the difference method is justified.

Key words. Stefan-type problem, free boundary, nonlinear Neumann condition, existence of solution, difference scheme, uniform convergence of approximations

AMS subject classifications. 65N06, 65N12, 35K20, 35K60, 35R35, 35A05

1. Introduction.

We consider the boundary-value problem,

$$\partial_t c(t,x) = \partial_{xx} c(t,x), \quad x \in \big(\rho(t), L\big), \quad t \in (0,T), \tag{1.1}$$

$$\partial_x c(t,L) = G\big(c(t,L)\big), \quad t \in [0,T], \tag{1.2}$$

$$\partial_x c\big(t,\rho(t)\big) = g\big(c(t,\rho(t))\big), \quad t \in [0,T], \tag{1.3}$$

$$c\big(t,\rho(t)\big)\dot{\rho} = -g\big(c(t,\rho(t))\big), \quad \rho(0) = \rho_0, \quad \rho(T) = 0, \tag{1.4}$$

$$c(0,x) = \varphi(x), \quad x \in [\rho_0, L], \quad 0 < \rho_0 < L. \tag{1.5}$$

The following assumptions are made: the functions $G(c)$ and $g(c)$ are defined for $c > 0$; the continuous derivatives $G'(c) < 0$, $g'(c) > 0$ for $c > 0$ exist; the conditions $G(1) > 0$, $G(\infty) < 0$, and $g(1) = 0$ hold; the function $\varphi(x)$ is defined for $x \in [\rho_0, L]$, $\varphi(x) > 1$, $G(\varphi(x)) > 0$ for $x \in [\rho_0, L]$, and $\varphi''(x)$ exists and is continuous in $[\rho_0, L]$. Note that the initial-boundary compatibility condition is included in the problem: conditions (1.2), (1.3) hold for $t = 0$. The following consequence can be derived.

PROPOSITION 1.1. *The initial distribution $\varphi(x)$ is not constant.*

Proof. If $\varphi(x) = \text{const}$, then $g(\varphi) = G(\varphi) = 0$ due to (1.2) and (1.3) and thus $\varphi = 1$; but $G(1) \neq 0$. ∎

Let us define the set $Y_\rho(T) \subset \mathbb{R}^2$; it consists of all (t,x) such that $t \in [0,T]$, $x \in [\rho(t), L]$. Its closure is $\bar{Y}_\rho(T)$. To solve the problem, we must find the number T, $\rho(t) \in C^1([0,T])$, and $c(t,x) \in C(Y_\rho(T))$. These functions must satisfy (1.1)–(1.5). If (1.1) is satisfied in a weak sense, then the solution obtained is called the weak solution.

This problem is a generalization of the model of isothermal hydriding of a metal particle under constant pressure [1]. Equation (1.1) is the diffusion equation; without loss of generality we assume that the diffusivity is unity. The nonlinear Neumann boundary condition (1.2) connects the diffusion flux near the surface with sorption and desorption on the surface. The stoichiometric concentration in hydride is unity. The condition $G(1) > 0$ means that the pressure is above equilibrium with respect to stoichiometric hydride. The condition (1.3)

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connects the diffusion flux on the phase boundary with the concentration near it and describes the hydride formation process. For stoichiometric concentration hydriding is impossible. The Stefan-type condition (1.4) is the conservation on the free boundary. The initial concentration (1.5) is between the stoichiometric and the equilibrium values.

The main difficulties are the free boundary and rather general nonlinear boundary conditions. Analytical solution methods [2] can hardly be applied to such problems. A lot of research has been devoted to the numerics of free boundary problems (e.g., [3, 4, 5, 6]), but little attention has been paid to diffusion boundary-value problems with free boundary in finite domains and with nonlinear boundary conditions. The aim of this paper is to apply the well-known idea of an implicit difference scheme with time steps dependent on the velocity of the free boundary (see [2] and references therein) to this class of problems and to prove the convergence to a classical solution. Therefore, we prove the existence of the solution in a constructive way. We prove the maximum principle for the discrete lattice problems and use it to construct a convergent sequence of approximations of a solution. The maximum principle for parabolic PDEs and the corresponding discrete systems is well-known [7, 8], but in our case it also holds on the boundary, i.e., boundary conditions also do not allow values of the solution to be too high. The restrictions are rather weak and have a physical meaning. Nevertheless, they are sufficient for the results obtained.

The structure of the paper is the following. First, we construct the difference scheme for this problem and prove a few statements for the lattice solution. Next, we obtain the sequences of continuous approximations to the free boundary and the concentration by linear interpolation. Then, we show that the sequence for the free boundary converges uniformly to some function $\rho(t)$, $\rho(T) = 0$ for some T; also the sequence for the concentration converges in $C(\bar{Y}_\rho(T))$. Next, we show that these functions are actually the classical solution of the problem. Therefore, we prove the existence of the classical solution of the nonlinear boundary-value problem with free boundary and additionally justify the difference scheme for the problem. The idea is from [2, 7].

The solution $c(t, x)$ must be positive (because it represents a concentration); moreover, $c(t, x) > 1$ because the concentration in hydride cannot be below the stoichiometric. We show that the solution indeed has these properties; see Theorem 3.4 below.

2. Difference approximations. Let us divide $[\rho_0, L]$ in M pieces of equal length $h = (L - \rho_0)/M$. In the sequel $h \to 0$ means $M \to \infty$. Let $I = \lfloor L/h \rfloor$ (integer part), $K = I - M$, and $\delta_h = L - Ih$. Choose any sequence K_n such that $K_0 = K$, for $n \geq 0$ either $K_{n+1} = K_n$ or $K_{n+1} = K_n + 1$. Let us denote $k_n = K_n - n$.

Now let us consider any spatially uniform lattice with the steps h and τ_n, $0 \leq n \leq N$, $0 \leq i \leq I$. Here N is the minimal N such that $\sum_0^N \tau_n \geq T$, $T > 0$ is some given time. Let the nodes of this lattice be (n, i); these are the points (t_n, x_i), $x_i = \delta_h + ih$, $t_0 = 0$, $t_{n+1} = t_n + \tau_n$, $n > 0$.

Let $\bar{D}_N$ be the lattice subset, such that, if $(n, i) \in \bar{D}_N$, then $0 \leq n \leq N$ and $i = k_n, k_n + 1, \ldots, I$. In other words, each succeeding layer contains either the same number of nodes (if $K_{n+1} = K_n + 1$) or one left node more (if $K_{n+1} = K_n$). Let D_N be the open subset; if $(n, i) \in D_N$ then $0 < n < N$ and $i = k_n + 1, k_n + 2, \ldots, I - 1$. We need one more lattice set $\tilde{D}_N$; it is $\bar{D}_N$ without the corner nodes $(0, K)$, $(0, I)$.

We denote the value of the lattice function f at the node (n, i) by f_n^i. Let us approximate the derivatives,

$$\partial_t c \approx \partial_\tau c_n^i = \frac{c_n^i - c_{n-1}^i}{\tau_{n-1}},\ \partial_x c \approx \partial_h c_n^i = \frac{c_n^{i+1} - c_n^i}{h},\ \partial_{xx} c \approx \partial_{hh} c_n^i = \partial_h(\partial_h c_n^{i-1}).$$

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Now replace the derivatives in (1.1)–(1.3) and (1.5) by the approximations,

$$\partial_\tau c_n^i = \partial_{hh} c_n^i, \quad (n,i) \in D_N, \tag{2.1}$$

$$\partial_h c_n^{I-1} = G(c_n^I), \quad 0 \le n \le N, \tag{2.2}$$

$$\partial_h c_n^{k_n} = g(c_n^{k_n}), \quad 0 \le n \le N, \tag{2.3}$$

$$c_0^i = \varphi(ih), \quad i = K, \dots, I. \tag{2.4}$$

This is a system of algebraic equations for the unknowns c_n^i, $(n,i) \in \bar{D}_N$. The sequence k_n and the steps h, τ_n are given.

3. The maximum principle for the lattice problem. Here we prove a few properties of the solution to the lattice problem (2.1)–(2.4). The technique is similar to the maximum principle for parabolic PDEs.

THEOREM 3.1. (*Maximum principle*). *Let the lattice function c_n^i be defined in $\bar{D}_N$, satisfy the system (2.1) in D_N, and its maximum or minimum be achieved at the node (n^*, i^*). Then either $n^* = 0$ or $i^* = I$ or $i^* = k_{n^*}$ or $c_n^i = \text{const}$ in $\tilde{D}_{n^*}$.*

Proof. Assume that the maximum (strict or not) is achieved at an inner node (n^*, i^*), $n^* > 0$, $k_{n^*} + 1 \le i^* \le I - 1$. Let us use (2.1), its left-hand side is obviously nonnegative, while the right-hand side is nonpositive. Thus $\partial_\tau c_{n^*}^{i^*} = \partial_{hh} c_{n^*}^{i^*} = 0$. Due to the fact that (n^*, i^*) is the maximum node, $c_{n^*}^{i^*\pm1} = c_{n^*}^{i^*}$ and $c_{n^*-1}^{i^*} = c_{n^*}^{i^*}$. The same argument applied to the nodes $(n^*, i^* \pm 1)$ yields $c_{n^*}^{i^*\pm2} = c_{n^*}^{i^*\pm1} = c_{n^*}^{i^*}$. Continuing the argument, we get $c_{n^*}^i = c_{n^*}^{i^*}$ for all $i = k_{n^*}, \dots, I$, i.e., the function is constant on the whole layer. As $c_{n^*-1}^{i^*} = c_{n^*}^{i^*}$, the same maximum is also obtained on the layer $n^* - 1$ and so the function is also constant on it. Continuing, we prove that $c_n^i = \text{const}$ on $\tilde{D}_{n^*}$. The proof for the minimum is similar. ☐

The theorem says that either $c_n^i = \text{const}$ in $\tilde{D}_{n^*}$ or the node $(n^*, i^*) \in \bar{D}_N \setminus D_N$.

COROLLARY 3.2. *Let the lattice function c_n^i be defined in $\bar{D}_N$ and satisfy the system (2.1), (2.4), its maximum or minimum (strict or not) be achieved at a node (n^*, i^*), and h be small enough. Then either $n^* = 0$ or $i^* = I$ or $i^* = k_{n^*}$.*

Proof. Due to (2.4) and Proposition 1.1, the function $\varphi(x)$ is not constant; then $c_0^i = \varphi(ih)$ is also not constant provided that h is small enough. Thus c_n^i is not constant in $\tilde{D}_n$ for any n. Theorem 3.1 provides the rest. ☐

THEOREM 3.3. *Let the lattice function c_n^i be defined in $\bar{D}_N$ and satisfy (2.1)–(2.4). Then $c_n^i < A$ in $\bar{D}_N$, the number $A > 0$ is such that $G(A) = 0$.*

Proof. It is sufficient to show the inequality for the maximum. The constant A is finite because $G(\infty) < 0$. As $G(\varphi) > 0$ and G is decreasing, $\varphi(x) < A$. The maximal value of c_n^i cannot be achieved at a node (n^*, k_{n^*}). Assume that $c_{n^*}^{k_{n^*}}$ is the maximum; therefore $c_{n^*}^{k_{n^*}+1} \le c_{n^*}^{k_{n^*}}$. The initial distribution $\varphi(x) > 1$ and thus $c_{n^*}^{k_{n^*}} > 1$. From (2.3) we know that $\partial_h c_{n^*}^{k_{n^*}} > 0$ and thus $c_{n^*}^{k_{n^*}+1} > c_{n^*}^{k_{n^*}}$. This shows that $c_{n^*}^{k_{n^*}}$ cannot be the maximal value. Assume that the maximal value of c_n^i is achieved at a node (n^*, I). The right-hand side of (2.2) is negative if $c_n^I > A$; therefore $\partial_h c_n^{I-1} < 0$. This means that $c_n^I < c_n^{I-1}$ and thus c_n^I cannot be maximal. If $c_n^I = A$ then the maximal value is achieved also at the inner node $(n, I-1)$. This is impossible due to Corollary 3.2. ☐

Note that the bound A depends only on $G(\cdot)$ and is independent of h, τ_n.

THEOREM 3.4. *Let the lattice function c_n^i be defined in $\bar{D}_N$ and satisfy (2.1)–(2.4). Then $c_n^i > 1$ in $\bar{D}_N$.*

Proof. It is sufficient to show the inequality for the minimum. For $n = 0$ it is given that $\varphi(x) > 1$. The minimal value $C \le 1$ cannot be achieved at a node (n^*, I). Assume the contrary; (2.2) yields $\partial_h c_{n^*}^{I-1} > 0$ (because $G(C) > 0$) and thus $c_{n^*}^I > c_{n^*}^{I-1}$. So

$c_{n^*}^I$ cannot be the minimum. Assume that the minimal value $C < 1$ is achieved at a node (n^*, k_{n^*}). From (2.3) we get $\partial_h c_{n^*}^{k_{n^*}} < 0$ (because $g(C) < 0$), i.e., $c_{n^*}^{k_{n^*}+1} < c_{n^*}^{k_{n^*}}$ and thus a contradiction. Let us consider the case of the minimal value $c_{n^*}^{k_{n^*}} = 1$. From (2.3) it follows that the minimum is also achieved at the inner node: $c_{n^*}^{k_{n^*}+1} = c_{n^*}^{k_{n^*}} = 1$. This is impossible due to Corollary 3.2. ◻

Note that the lattice solution $c_n^i > 1$ in $\bar{D}_N$ and thus it is positive.

THEOREM 3.5. (*Uniqueness*) *Let c_n^i and w_n^i be two solutions to system (2.1)–(2.4) in $\bar{D}_N$. Then $c_n^i = w_n^i$ in $\bar{D}_N$.*

Proof. Consider the lattice function $w_n^i = c_n^i - u_n^i$. We need to prove that $w_n^i = 0$ in $\bar{D}_N$. Suppose the contrary: let $w_n^i > 0$ at some node (n, i).

The function w_n^i satisfies (2.1) due to linearity. Therefore, Corollary 3.2 guarantees that the positive maximum is achieved on the boundary of $\bar{D}_N$. But $w_0^i = 0$, so the maximum cannot be achieved if $n = 0$.

Note that w_n^i satisfies the condition

$$\partial_h w_n^{k_n} = g\big(c_n^{k_n}\big) - g\big(u_n^{k_n}\big) = g'(R_1) w_n^{k_n}, \quad R_1 \in \big[u_n^{k_n}, c_n^{k_n}\big].$$

If the maximum is achieved at a node (n, k_n), then the left-hand side is nonpositive while the right-hand side is greater than zero (remember that $g' > 0$). The contradiction means that a maximum is impossible.

Finally, w_n^i satisfies the condition

$$\partial_h w_n^{I-1} = G\big(c_n^I\big) - G\big(u_n^I\big) = G'(R_2) w_n^I, \quad R_2 \in \big[u_n^I, c_n^I\big].$$

If the maximum is achieved at the node (n, I), then the left-hand side is nonnegative, while the right-hand side is less than zero ($G' < 0$). A maximum is impossible.

The contradiction implies that no positive maximum of w_n^i can be achieved in $\bar{D}_N$. Thus $c_n^i = u_n^i$ in $\bar{D}_N$. ◻

Let us consider the lattice set $\bar{D}'_N$: if $(n, i) \in \bar{D}'_N$ then $0 \le n \le N$, $k_n \le i \le I - 1$. In other words, the set contains one node less at each layer compared to $\bar{D}_N$. Also we will consider the subset D'_N with the nodes (n, i), $0 < n < N$, $k_n + 1 \le i \le I - 2$. The set $\tilde{D}'_N$ is equal to $\bar{D}'_N$ without the corner nodes $(0, K)$ and $(0, I - 1)$.

Let c_n^i satisfy the system (2.1)–(2.4) in $\bar{D}_N$. The lattice derivative $\partial_h c_n^i$ is defined as a lattice function in $\bar{D}'_N$ and satisfies (2.1) in D'_N. Thus it obeys Theorem 3.1: if its minimum or maximum is achieved at the node (n^*, i^*), then either $n^* = 0$ or $i^* = I - 1$ or $i^* = k_{n^*}$ or it is constant in $\tilde{D}'_{n^*}$.

THEOREM 3.6. *Let c_n^i satisfy (2.1)–(2.4) in $\bar{D}_N$. The lattice derivative $\partial_h c_n^i$ is bounded: $|\partial_h c_n^i| < B$ in $\bar{D}'_N$. The constant B does not depend on h and τ_n. If additionally $\varphi'(x) > 0$ on $[\rho_0, L]$ then $\partial_h c_n^i > 0$ in $\bar{D}'_N$.*

Proof. Extremal values of $\partial_h c_n^i$ cannot be achieved in D'_N due to the maximum principle. Therefore, we only need to check if the values are bounded at the nodes $(0, i)$, $(n, I-1)$, and (n, k_n). Due to (2.4) $\partial_h c_0^i = \varphi'(x_i + \theta)$, $0 \le \theta \le h$, is bounded for all $i = K, \dots, I - 1$. From (2.2) and Theorems 3.3 and 3.4, we have $\partial_h c_n^{I-1} = G(c_n^I) \in \big(0, G(1)\big)$. Finally, (2.3) and Theorems 3.3 and 3.4 imply $\partial_h c_n^{k_n} = g\big(c_n^{k_n}\big) \in \big(0, g(A)\big)$. ◻

Let us construct the lattice subset $\bar{D}''_N \subset \bar{D}_N$ in the following way: a node $(n, i) \in \bar{D}_N$ belongs to $\bar{D}''_N$ if the node $(n - 1, i)$ belongs to $\bar{D}_N$. One can see that in $\bar{D}''_N$ the index $n > 0$ (i.e., the layer $n = 0$ is not contained); also the nodes (n, k_n) are not contained if $K_n = K_{n-1}$. Therefore this subset is generated by some sequence K''_n, $n \ge 1$. Denote $k''_n = K''_n - n$. Let us consider also the subsets D''_N and $\tilde{D}''_N$ similarly to D_N and $\tilde{D}_N$.

Let c_n^i satisfy the system (2.1)–(2.4) in $\bar{D}_N$. The lattice derivative $\partial_\tau c_n^i$ is defined as a lattice function on $\bar{D}''_N$ and satisfies (2.1) in D''_N. Thus it obeys Theorem 3.1; if its minimum

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or maximum is achieved at the node (n^*, i^*) then either $n^* = 1$ or $i^* = I$ or $i^* = k''_{n^*}$ or it is constant in $\tilde{D}''_N$.

THEOREM 3.7. *Let c_n^i satisfy (2.1)–(2.4) in $\bar{D}_N$. The lattice derivative $\partial_\tau c_n^i$ is bounded: $|\partial_\tau c_n^i| < Z$ in $\bar{D}''_N$. The constant Z does not depend on h and τ_n.*

Proof. Extremal values of $\partial_h c_n^i$ cannot be achieved in D''_N due to the maximum principle. Therefore, we only need to check if the values of $\partial_\tau c_n^i$ are bounded at the nodes (n, I), (n, k''_n), and $(0, i)$.

Consider two nodes $(n+1, I)$ and (n, I), $n \geq 0$. Due to (2.2),

$$c_{n+1}^I - c_{n+1}^{I-1} = hG(c_{n+1}^I), \quad c_n^I - c_n^{I-1} = hG(c_n^I).$$

Substract the second expression from the first one and divide by τ_n,

$$\partial_\tau c_{n+1}^I - \partial_\tau c_{n+1}^{I-1} = hG'(Q_1)\partial_\tau c_{n+1}^I, \quad Q_1 \in [c_n^I, c_{n+1}^I].$$

As $G' < 0$, the positive maximum and negative minimum of the function $\partial_\tau c_n^i$ cannot be achieved for $i = I$, otherwise the contradiction appears.

Now consider two nodes $(n+1, k''_{n+1})$ and (n, k''_n), $n \geq 0$. There can be two cases. First, let us study the case $K''_{n+1} = K''_n + 1$. Due to (2.3),

$$c_{n+1}^{k''_n+1} - c_{n+1}^{k''_n} = hg\left(c_{n+1}^{k''_n}\right), \quad c_n^{k''_n+1} - c_n^{k''_n} = hg\left(c_n^{k''_n}\right).$$

Substract the second expression from the first one and divide by τ_n,

$$\partial_\tau c_{n+1}^{k''_n+1} - \partial_\tau c_{n+1}^{k''_n} = hg'(Q_2)\partial_\tau c_{n+1}^{k''_n}, \quad Q_2 \in \left[c_n^{k''_n}, c_{n+1}^{k''_n}\right].$$

As $g' > 0$, the positive maximum and negative minimum of the function $\partial_\tau c_n^i$ cannot be achieved at the node (n, k''_n) if $K''_n = K''_{n-1} + 1$.

Second, we study the case $K''_{n+1} = K''_n$. Due to (2.3)

$$c_{n+1}^{k''_n} - c_{n+1}^{k''_n-1} = hg\left(c_{n+1}^{k''_n-1}\right), \quad c_n^{k''_n+1} - c_n^{k''_n} = hg\left(c_n^{k''_n}\right).$$

Substract the first expression from the second one,

$$\left(c_{n+1}^{k''_n-1} - c_n^{k''_n}\right) + \left(c_n^{k''_n+1} - c_{n+1}^{k''_n}\right) = -hg'(Q_3)\left(c_{n+1}^{k''_n-1} - c_n^{k''_n}\right), \quad Q_3 \in \left[c_n^{k''_n}, c_{n+1}^{k''_n-1}\right].$$

Now let us transform the first bracket on the left-hand side,

$$c_{n+1}^{k''_n-1} - c_n^{k''_n} = c_{n+1}^{k''_n-1} - c_{n+1}^{k''_n} + c_{n+1}^{k''_n} - c_n^{k''_n} = -\partial_h c_{n+1}^{k''_n-1} h + \partial_\tau c_{n+1}^{k''_n}\tau_n,$$

and the second bracket on the left-hand side,

$$c_n^{k''_n+1} - c_{n+1}^{k''_n} = \partial_h c_{n+1}^{k''_n} h - \partial_\tau c_{n+1}^{k''_n+1}\tau_n.$$

The bracket on the right-hand side equals the first one on the left-hand side. Therefore,

$$(1 + hg'(Q_3))\partial_\tau c_{n+1}^{k''_n} = \partial_\tau c_{n+1}^{k''_n+1} + \frac{h}{\tau_n}\left(\partial_h c_{n+1}^{k''_n-1} - \partial_h c_{n+1}^{k''_n}\right) + \frac{h^2}{\tau_n} g'(Q_3)\partial_h c_{n+1}^{k''_n-1}.$$

The big bracket equals $-\partial_{hh} c_{n+1}^{k''_n} h = -\partial_\tau c_{n+1}^{k''_n} h$ (we have used (2.1)). Thus,

$$(1 + hg'(Q_3))\partial_\tau c_{n+1}^{k''_n} = \partial_\tau c_{n+1}^{k''_n+1} + \frac{h^2}{\tau_n}\left(g'(Q_3)\partial_h c_{n+1}^{k''_n} - \partial_\tau c_{n+1}^{k''_n}\right).$$

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Then due to boundedness, $\partial_h c_n^i \le B$,

$$\big(1 + hg'(Q_3)\big)\partial_\tau c_{n+1}^{k''_n} \le \partial_\tau c_{n+1}^{k''_n+1} + \frac{h^2}{\tau_n}\Big(g'(Q_3)B - \partial_\tau c_{n+1}^{k''_n}\Big).$$

Now we see that if $\partial_\tau c_{n+1}^{k''_n}$ is the maximal positive value, then it is less than $\max\limits_{[1,A]}(g')B$. Otherwise, the bracket in the right-hand side is negative and thus

$$\partial_\tau c_{n+1}^{k''_n} \le \partial_\tau c_{n+1}^{k''_n+1}.$$

A similar argument shows that the minimal possible value is also bounded.

Now let us study the case $n = 1$. Let $\varepsilon^i = c_1^i - c_0^i$ and consider (2.1) for $n = 1$, $K \le i \le I - 1$:

$$\partial_\tau c_1^i = \frac{c_1^{i-1} - 2c_1^i + c_1^{i+1}}{h^2} = \frac{c_0^{i-1} - 2c_0^i + c_0^{i+1}}{h^2} + \frac{\varepsilon^{i-1} - 2\varepsilon^i + \varepsilon^{i+1}}{h^2}.$$

But $c_0^{i-1} - 2c_0^i + c_0^{i+1} = h^2\varphi''(x_i) + o(h^2)$ and thus the first term in the right-hand side is bounded. Besides $\partial_\tau c_1^i = \varepsilon^i/\tau_0$. Therefore,

$$\tau_0^{-1}\varepsilon^i = h^{-2}\big(\varepsilon^{i-1} - 2\varepsilon^i + \varepsilon^{i+1}\big) + R(i).$$

Here $R(i)$ is bounded independently on h and τ_0. Let the function $\partial_\tau c_n^i$ reach a positive maximum at the node $(1, i^*)$; then ε^{i^*} also reaches the positive maximum. But the first term in the right-hand side is negative; so $\tau_0^{-1}\varepsilon^i \le R(i)$ and thus is bounded. A similar argument applies to the negative minimum.

Let us sum this all up. Minimal and maximal values of the lattice function $\partial_\tau c_n^i$ in $\bar{D}''_N$ are achieved at the nodes (n^*, i^*) for either $n^* = 1$ or $i^* = I$ or $i^* = k''_{n^*}$. But these extremal values are bounded independently on the steps; therefore there exists Z such that $|\partial_\tau c_n^i| \le Z$ in $\bar{D}''_N$. ∎

COROLLARY 3.8. *The second lattice derivative $\partial_{hh} c_n^i$ is bounded independently of the steps at nodes where it is defined.*

COROLLARY 3.9. *If the initial distribution has a positive second derivative $\varphi''(x) > 0$ and the step h is sufficiently small, then $\partial_\tau c_n^i > 0$ in $\bar{D}''_N$.*

COROLLARY 3.10. *Let $\varphi'(x) > 0$ and $\varphi''(x) > 0$ and the step h be sufficiently small. Then $0 < \partial_h c_n^i < B$ in $\bar{D}'_N$ and $B = \partial_h c_0^{I-1}$.*

Proof. As $\partial_\tau c_n^i > 0$, then also $\partial_{hh} c_n^i > 0$ at nodes where it is defined. This implies, in particular, $\partial_h c_n^{k_n} < \partial_h c_n^{k_n+1}$ and therefore the maximal value of $\partial_h c_n^i$ cannot be achieved at a node (n, k_n). As $\partial_\tau c_n^i > 0$, c_n^I increases; due to monotonicity of the function G the right-hand side of (1.2) decreases. Thus if the maximal value of $\partial_h c_n^i$ is achieved at a node (n, I), then $n = 0$. The only possibility for the maximum is the node $(0, I - 1)$. ∎

4. Choosing the time step. Up to this point we considered the given lattice; the spatial step h, the time steps τ_n, the sequence K_n (it generates the subset $\bar{D}_N$), and the time T were fixed. But τ_n and K_n have to be determined. Some equations must be added to the system (2.1)–(2.4) to find not only unknown c_n^i but also unknown τ_n and K_n.

Let us consider the lattice analogue of the Stefan condition (1.4),

$$\partial_\tau \rho_{n+1} = \frac{\rho_{n+1} - \rho_n}{\tau_n} = -\frac{g\big(c_n^{k_n}\big)}{c_n^{k_n}}.$$

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We have already proved that $c_n^{k_n} > 1$ and thus the shift of the free boundary is negative: $\rho_{n+1} - \rho_n < 0$. In order to make the absolute value of this shift equal h (up to the error of approximation), we need to choose the special τ_n,

$$\tau_n = \frac{c_n^{k_n}}{g\big(c_n^{k_n}\big)} h.$$

However, it can turn out that $c_n^{k_n}$ is close to unity, so $g\big(c_n^{k_n}\big)$ is too small and then τ_n is too large. If τ_n does not tend to zero as $h \to 0$, then there is no approximation.

From (1.4) it follows that the boundary moves slowly when the concentration near the boundary is close to unity: $\dot{\rho} \approx -g'\big(c_n^{k_n}\big)\big(c_n^{k_n} - 1\big)$. Therefore let us assume that for small $c_n^{k_n}$, the boundary does not move. Let us consider $c_n^{k_n}$ small if

$$g\big(c_n^{k_n}\big) < \varphi'(\rho_0)\sqrt{h}. \tag{4.1}$$

The left-hand side is positive. Let the step h obey the inequality $h \leq 1$. The reason is to guarantee that the initial distribution is not small.

Summing this up, we choose the steps τ_n as follows,

$$\tau_n = \begin{cases} \dfrac{c_n^{k_n}}{g\big(c_n^{k_n}\big)} h, & \text{if} \quad g\big(c_n^{k_n}\big) \geq \varphi'(\rho_0)\sqrt{h}, \\ \dfrac{g^{-1}\big(\varphi'(\rho_0)\sqrt{h}\big)}{\varphi'(\rho_0)}\sqrt{h} < \Gamma\sqrt{h} = \bar{\tau}, & \text{otherwise}. \end{cases} \qquad 0 \leq n \leq N-1, \tag{4.2}$$

Here g^{-1} is for the inverse function, $\Gamma = \mathrm{const}$ is independent of h. Note that bounds for the time step $\tau_n > h/g(A)$, $\tau_n < \bar{\tau} = O(\sqrt{h})$ hold.

In the first, case the boundary shifts left one step h during a time step; in the second case, it remains motionless. In other words, in the first case we add a node to the new layer, while in the second case we do not. Therefore,

$$K_{n+1} = \begin{cases} K_n, & \text{if} \quad g\big(c_n^{k_n}\big) \geq \varphi'(\rho_0)\sqrt{h}, \\ K_n + 1, & \text{otherwise}. \end{cases} \qquad 0 \leq n \leq N-1, \tag{4.3}$$

The system (2.1)–(2.4), (4.2), and (4.3) is called the system $(*)$.

PROPOSITION 4.1. *Let c_n^i satisfy the system $(*)$ in $\bar{D}_1$. Then $\partial_h c_n^i \neq \mathrm{const}$ in $\bar{D}'_N$.*

Proof. Due to $h < 1$ the initial value $\varphi(\rho_0)$ is not small and thus $K_1 = K_0 = K$. Thus the layer $n = 1$ has one node more compared to the layer $n = 0$. Assume that the lattice derivative $\partial_h c_n^i$ is constant in $\bar{D}'_1$. Then due to (2.4) $\partial_h c_n^i = \varphi'(\rho_0)$ in $\bar{D}'_1$. In particular, $\partial_h c_0^K = \partial_h c_1^{K-1}$ and from (2.3) we have $g\big(c_0^K\big) = g\big(c_1^{K-1}\big)$. As $g(c)$ is monotonic, this means $c_0^K = c_1^{K-1}$. Thus $c_1^K = c_0^K + \varphi'(\rho_0)h$. In the similar way, $c_1^{K+i} = c_0^K + \varphi'(\rho_0)(i+1)h$. Thus $c_1^N = c_0^K + \varphi'(\rho_0)(N-K+1)h$. As the derivative is constant, $c_0^N = c_0^K + \varphi'(\rho_0)(N-K)h \neq c_1^N$. However, due to (2.2) $G\big(c_0^N\big) = G\big(c_1^N\big)$ and, thus, $c_0^N = c_1^N$ because $G(c)$ is monotonic. This contradiction shows that $\partial_h c_n^i$ cannot be constant in $\tilde{D}'_1$ and thus in $\bar{D}'_N$ for any $N \geq 1$. $\square$

5. Solving the system. We are going to present an algorithm for the solution of the system $(*)$. Thus we will prove that it has a solution. A solution is a set τ_n for $0 \leq n \leq N-1$, K_n for $0 \leq n \leq N$, c_n^i for $0 \leq n \leq N$, $k_n \leq i \leq I$ for given natural M; $h < 1$, I, K, N, and T are uniquely determined.

Let us develop a sweep method to obtain c_n^i when the c_{n-1}^i are already known. Denote $X = c_n^{k_n}$, $Y = c_n^I$. Express all c_n^i, $i = k_n + 1, \ldots, I-1$ via c_n^{i+1} and X linearly with unknown coefficients,

$$c_n^i = a_i c_n^{i+1} + b_i + d_i X. \tag{5.1}$$

Substitute (5.1) into (2.1) instead of c_n^{i-1} for $i = k_n + 2, \ldots, I-1$. The result is

$$c_n^i = \frac{c_n^{i+1} + S_n c_{n-1}^i + b_{i-1} + d_{i-1}X}{2 + S_n - a_{i-1}}.$$

Here $S_n = h^2/\tau_{n-1}$. Then

$$a_i = (2 + S_n - a_{i-1})^{-1}, \quad b_i = a_i(S_n c_{n-1}^i + b_{i-1}), \quad d_i = a_i d_{i-1}. \tag{5.2}$$

This are the recurrent sequences. To get the initial values consider (2.1) for $i = k_n + 1$,

$$c_n^{k_n+1} = \frac{c_n^{k_n+2} + S_n c_{n-1}^{k_n+1} + X}{2 + S_n}.$$

Hence, $a_{k_n+1} = d_{k_n+1} = (2 + S_n)^{-1}$, $b_{k_n+1} = a_{k_n+1} S_n c_{n-1}^{k_n+1}$.

Now express c_n^i, $i = k_n + 1, \ldots, I-1$ via c_n^{i-1} similarly,

$$c_n^i = A_i c_n^{i-1} + B_i + D_i Y. \tag{5.3}$$

Analogously,

$$A_i = (2 + S_n - A_{i+1})^{-1}, \quad B_i = A_i(S_n c_{n-1}^i + B_{i+1}), \quad D_i = A_i D_{i+1},$$

with initial values $A_{I-1} = D_{I-1} = (2 + S_n)^{-1}$, $B_{I-1} = A_{I-1} S_n c_{n-1}^{I-1}$.

PROPOSITION 5.1. *The following inequalities hold for* $k_n + 1 \leq i \leq I - 1 : a_i \in (0, 1)$, $a_{i+1} > a_i$, $d_i \in (0, 0.5)$, $d_{i+1} < d_i$, $b_i > 0$, $a_i < 1 - \Gamma_1 h^{\frac{3}{4}}$ *for some constant* $0 < \Gamma_1 < 1$. *The same inequalities hold for* A_i, B_i, D_i.

Proof. The first five inequalities are proven by induction; obviously they are true for $i = k_n + 1$; if they hold for some i then (5.2) shows that they also do for $i + 1$.

The sequence a_i increases and is bounded; therefore it has an upper bound. To calculate it find the fixed point a of the function $a_i(a_{i-1})$, i.e., solve the equation $a^2 - (2+S_n)a + 1 = 0$. It has a real root a from $(0, 1)$. If $a_i = a$ then $a_{i+1} = a$. As $a_{k_n+1} < a$, so $a_i < a$, $1 - a_i > 1 - a$. Let us estimate

$$\begin{aligned}
1 - a &= \frac{\sqrt{4S_n + S_n^2} - S_n}{2} = \frac{2S_n}{\sqrt{4S_n + S_n^2} + S_n} = \frac{2h^2}{\sqrt{4h^2\tau_{n-1} + h^4} + h^2} = \\
&= \frac{2h}{\sqrt{4\tau_{n-1} + h^2} + h} > \frac{2h}{\sqrt{4\bar{\tau} + h^2} + h} = \frac{2h}{\sqrt{4\Gamma\sqrt{h} + h^2} + h} > \\
&> \frac{h}{\sqrt{4\Gamma\sqrt{h} + h^2}} > \frac{h^{3/4}}{\sqrt{4\Gamma + h^{3/2}}} > \frac{h^{3/4}}{\sqrt{4\Gamma + 1}} = \Gamma_1 h^{\frac{3}{4}}.
\end{aligned}$$

This finishes the proof. The proof for A_i, B_i, D_i is similar. ☐

Substitute (5.1) for $i = I - 1$ and (5.3) for $i = k_n + 1$ into (2.2) and (2.3), respectively,

$$Y(1 - a_{I-1}) - hG(Y) = b_{I-1} + d_{I-1}X, \tag{5.4}$$

$$X(1 - A_{k_n+1}) + hg(X) = B_{k_n+1} + D_{k_n+1}Y. \tag{5.5}$$

This is a system of two non-linear equations with two unknowns, X and Y.

We have proved that a solution to the lattice problem (2.1)–(2.4) with any steps h and τ_n is greater than unity and bounded independently of the step sizes. Therefore we can suppose without loss of generality that the function $g(c)$ grows faster than c: let $g(c)/c \to \infty$ as

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$c \to \infty$. For technical purposes we may need $G(c)$ for negative c; suppose that it remains continuous and monotonic and thus $G(c) > 0$ for $c < 0$.

THEOREM 5.2. *The system of equations* (5.4) *and* (5.5) *has a solution*; *if h is sufficiently small, then the solution is unique.*

Proof. Let us express Y as a function of X defined by (5.5). We see that $Y(0) < 0$ because $g(1) = 0$ and increases (and thus $g(0) \le 0$), $B_i > 0$, $D_i > 0$. On the other hand, $Y(+\infty) = +\infty$ because $1 - A_i > 0$. Moreover, $Y(X)$ grows faster than X.

Now substitute $Y(X)$ into (5.4) and consider the continuous function

$$F(X) = Y(X)(1 - a_{I-1}) - hG\big(Y(X)\big) - b_{I-1} - d_{I-1}X.$$

If $F(X^*) = 0$, then the pair $(X^*, Y(X^*))$ is a solution to the system of equations (5.4) and (5.5). To prove that $F(X)$ has a zero, note that $F(0) < 0$ (because $a_i < 1$, G is decreasing, $b_i > 0$, $d_i > 0$) and $F(\infty) = \infty$ (because $a_i < 1$ and $Y(X)$ grows faster than X). Hence, there exist $X^* \ge 0$ and $Y^* = Y(X^*)$, such that equations (5.4) and (5.5) are satisfied.

To prove the uniqueness, let us show that the derivative $F'(X) > 0$,

$$\begin{aligned} D_{k_n+1}F'(X) = D_{k_n+1}Y'(X)\Big(1 - a_{I-1} - hG'\big(Y(X)\big)\Big) - D_{k_n+1}d_{I-1} = \\ \Big((1 - A_{k_n+1}) + hg'(X)\Big)\Big(1 - a_{I-1} - hG'\big(Y(X)\big)\Big) - D_{k_n+1}d_{I-1}. \end{aligned}$$

To prove that $F'(X) > 0$, it is sufficient to show that

$$1 - A_{k_n+1} > D_{k_n+1}, \quad 1 - a_{I-1} > d_{I-1}.$$

These inequalities are proved similarly, so let us prove the second one,

$$1 - a_{I-1} > \Gamma_1 h^{\frac{3}{4}}, \quad d_{I-1} = d_{k_n+1} \prod_{m=k_n+2}^{I-1} a_m < \frac{1}{2}\left(1 - \Gamma_1 h^{\frac{3}{4}}\right)^{I-k_n-2}.$$

Suppose that h is small enough so that $2\big(1 - \Gamma_1 h^{\frac{3}{4}}\big)^2 > 1$. Then

$$d_{I-1} < \left(1 - \Gamma_1 h^{\frac{3}{4}}\right)^{I-k_n} < \left(1 - \Gamma_1 h^{\frac{3}{4}}\right)^{I-K} = \left(1 - \Gamma_1 h^{\frac{3}{4}}\right)^{\frac{L-\rho_0}{h}}.$$

The function $f(z) = (1 - z)^{\frac{1}{z}}$ is decreasing. Therefore, $f(z) < f(0) = \exp(-1)$. Thus,

$$d_{I-1} < \left(\left(1 - \Gamma_1 h^{\frac{3}{4}}\right)^{\frac{1}{\Gamma_1 h^{\frac{3}{4}}}}\right)^{\frac{(L-\rho_0)\Gamma_1}{h^{\frac{1}{4}}}} < \exp\left(-\frac{(L-\rho_0)\Gamma_1}{h^{\frac{1}{4}}}\right) = o(h^\alpha)$$

for any $\alpha > 0$. Hence, for sufficiently small h, we have $d_{I-1} < \Gamma_1 h^{\frac{3}{4}}$. ∎

Note that a small h is not necessary for the uniqueness of the solution.

Here we present the algorithm:

1. Let $n = 0$. Define $K_0 = K$. For $K_0 \le i \le I$ calculate c_0^i using (2.4).
2. Find τ_n from (4.2). Obviously $h < \tau_n \le \bar{\tau}$.
3. Detemine K_{n+1} from (4.3) and calculate $k_{n+1} = K_{n+1} - (n + 1)$.
4. If $k_{n+1} = 0$ then stop: the problem is solved because the boundary has reached zero. Assign $T = \sum \tau_n$, N.
5. Increase n by one.

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6. Solve equations (5.4) and (5.5) simultaneously to obtain X and Y.
7. Using (5.1) and the computed a_i, b_i, d_i, $X = c_n^{k_n}$, $Y = c_n^I$, calculate c_n^i one by one for $i = I-1, I-2, \ldots, k_n+1$. It is also possible to use (5.3).
8. Go to step 2.

We have not proved that the determined $X > 1$ and $Y > 1$; but this is true because the constructed solution obeys Theorem 3.4.

THEOREM 5.3. *Provided that h is sufficiently small, the algorithm terminates after a finite number of steps.*

Proof. Suppose that the algorithm never stops; the boundary moves only in a finite number of steps. Thus, after the finite number of steps the boundary does not move ($k_n = \mathrm{const}$ for sufficiently large n). Let us see how the amount of matter changes,

$$\sum_{i=k_n+1}^{I-1} c_n^i h - \sum_{i=k_n+1}^{I-1} c_{n-1}^i h = \sum_{i=k_n+1}^{I-1} \partial_\tau c_n^i \bar{\tau} h = \sum_{i=k_n+1}^{I-1} \partial_{hh} c_n^i h\bar{\tau} = \sum_{i=k_n+1}^{I-1} \partial_h \big(\partial_h c_n^{i-1}\big) h\bar{\tau}$$
$$= \sum_{i=k_n+1}^{I-1} \big(\partial_h c_n^i - \partial_h c_n^{i-1}\big)\bar{\tau} = \big(\partial_h c_n^{I-1} - \partial_h c_n^{k_n}\big)\bar{\tau}.$$

The boundary does not move, so $c_n^{k_n}$ is small, and thus

$$g(c_n^{k_n}) < \varphi'(\rho_0)\sqrt{h} < \varphi'(\rho_0) \quad \text{and} \quad c_n^{k_n} < g^{-1}(\varphi'(\rho_0)) = \varphi(\rho_0).$$

It is necessary that $\partial_h c_n^{I-1} - \varphi'(\rho_0)\sqrt{h} \to 0$, otherwise the amount $\sum\limits_{i=k_n+1}^{I-1} c_n^i h$ grows to infinity and some c_n^i become greater than A for large n. Thus if n is large,

$$G(c_n^I) = \partial_h c_n^{I-1} \approx \varphi'(\rho_0)\sqrt{h} \quad \text{and} \quad c_n^I \approx G^{-1}(\varphi'(\rho_0)\sqrt{h}) > \varphi(\rho_0) + \epsilon.$$

The last inequality holds for sufficiently small h and some $\epsilon > 0$. Hence, $c_n^I - c_n^{k_n} > \epsilon$.

On the other hand, if $\partial_h c_n^{k_n+1}$ and $\partial_h c_n^{I-1}$ remain small, then $\partial_h c_n^i$ for all $i = k_n, \ldots, I-1$ become small for sufficiently large n. This follows from the maximum principle. So we can assume that $|\partial_h c_n^i| < \varphi'(\rho_0)\sqrt{h}$ for $i = k_n, \ldots, I-1$. Then

$$c_n^I - c_n^{k_n} = \sum_{i=k_n}^{I-1} \partial_h c_n^i h < \sum_{i=1}^{I} \varphi'(\rho_0) h\sqrt{h} = \varphi'(\rho_0) h^{\frac{3}{2}} I < \varphi'(\rho_0) L\sqrt{h}.$$

If h is sufficiently small, this is below any $\epsilon > 0$. Thus we have the contradiction. □

It is easy to show that the time $T(h) = \sum \tau_n$ is also finite and, moreover, bounded for all h: $T(h) \le \bar{T}$ for some $\bar{T}$.

6. Order of approximation. Let us suppose that the classical smooth solution $\rho(t)$, $c(t,x) > 1$ to the boundary-value problem (1.1)–(1.5) exists. We need to see how large the error is if we substitute it into the system $(*)$.

First, we see that, for all n, $\tau_n \to 0$ as $h \to 0$, and thus, the rate of convergence is at least $\bar{\tau} = O(\sqrt{h})$. Consider the equation $\partial_\tau c_n^i - \partial_{hh} c_n^i = \Psi_n^i$. If c_n^i is a solution to (2.1) then $\Psi_n^i \equiv 0$ in D_N. Substitute the values of the exact solution $c(t_n, x_i)$ at nodes of the lattice subset $\bar{D}_N$ into the left-hand side. Then in general $\Psi_n^i \ne 0$ is some lattice function called the discrepancy. Let Ψ denote the maximum of the absolute value of the Ψ_n^i on D_N. Using the Taylor expansion for the exact solution and the diffusion equation (1.1), we obtain $\Psi = O(h^2, \bar{\tau}) = O(\sqrt{h})$. These are standard arguments of the theory of numerical methods, so the details are omitted. In a similar way, we substitute the exact solution into (2.2) and (2.3). The discrepancy turns out to be $O(h)$. The initial condition (2.4) is satisfied precisely.

Let us recall how we approximated the Stefan condition (1.4),

$$\partial_\tau \rho_{n+1} = \frac{\rho_{n+1} - \rho_n}{\tau_n} = -\frac{g\big(c_n^{k_n}\big)}{c_n^{k_n}}, \quad \text{if} \quad g\big(c_n^{k_n}\big) \geq \varphi'(\rho_0)\sqrt{h}, \tag{6.1}$$

and zero otherwise. Substitute the exact solution $\rho(t)$, $c\big(t, \rho(t)\big)$ with a discrepancy Ψ_n and apply the Stefan condition (1.4),

$$O(\bar\tau) + \Psi_n = \frac{g\Big(c\big(t_n, \rho(t_n)\big)\Big)}{c\big(t_n, \rho(t_n)\big)} \leq \varphi'(\rho_0)\sqrt{h}, \quad \text{if} \quad g\Big(c\big(t_n, \rho(t_n)\big)\Big) < \varphi'(\rho_0)\sqrt{h},$$

and zero otherwise. In both cases $\Psi_n = O\big(\sqrt{h} + \bar\tau\big) = O\big(\sqrt{h}\big)$. Thus the total discrepancy and the order of approximation of the scheme is $O\big(\sqrt{h}\big)$.

The order of approximation cannot be made better than $\sqrt{h}$ by just choosing the condition (4.1) in the form $g\big(c_n^{k_n}\big) < \varphi'(\rho_0)h^{1-\epsilon}$ with $\epsilon > 0.5$. If we do so then $\tau_n \leq \bar\tau = O\big(h^\epsilon\big)$. The discrepancy of the Stefan condition and thus the total discrepancy will become worse, $O(h^{1-\epsilon})$.

7. Convergence of approximations. In the remainder of the paper, we assume that h is sufficiently small.

If an h is chosen, one can determine a solution using the presented algorithm. The solution is the set of T, τ_n for $0 \leq n \leq N-1$, $\bar D_N$, and c_n^i in $\bar D_N$. Theorem 3.5 guarantees that if the domains $\bar D_n$ are the same for two solutions, they coincide.

Construct the piecewise linear continuous time function $\rho_h(t)$ by connecting the points (t_n, x_{k_n}) (linear interpolation). Being piecewise linear $\rho_h(t)$ has a piecewise constant derivative between the nodes; let us estimate it. The difference $x_{k_{n+1}} - x_{k_n}$ is either zero (if $K_{n+1} = K_n + 1$) or $-h$ (if $K_{n+1} = K_n$). The difference $t_{n+1} - t_n = \tau_n$. We know that $\tau_n \geq h/g(A)$. Thus the derivative between the nodes belongs to $[-g(A), 0]$ for any h. The function $\rho_h(t) \in [0, \rho_0]$ for all h and is defined for $t \in [0, T(h)]$. Let us expand it to $[0, \bar T]$ being continuous and constant for $t > T$.

Now let us consider a sequence $h_j \to 0$. The functions $\rho_{h_j}(t)$ on $[0, \bar T]$ are uniformly bounded and equicontinuous; due to the Arzela–Ascoli theorem a uniformly convergent subsequence can be selected (but may be not unique). Denote this subsequence again by h_j and its limit by $\rho(t)$. The functions $\rho_{h_j}(t)$ are all nonnegative, uniformly bounded by $\rho_0 < L$, and non-increasing; thus $\rho(t)$ is also nonnegative, bounded by ρ_0, and does not increase. Also $\rho(T) = 0$ for some $T \in [0, \bar T]$. This is the continuous free boundary.

Now define the lattice function c_n^i at the nodes $(n, i) \notin \bar D_N$: let $c_n^{k_n - 1} = c_n^{k_n} - \partial_h c_n^{k_n} h$, at other nodes $(n, i) \notin \bar D_N$ let $c_n^i = c_n^{k_n - 1}$. The continuous approximations $\psi_h(t, x)$ in the rectangle $\aleph = [0, T] \times [0, L]$ are constructed in the following way. Let $\psi_h(t_n, x_i) = c_n^i$ at the nodes (n, i). For each n we define $\psi_h(t_n, x)$ to be a polynomial of the fifth order $P_{n,i}(x)$ on each segment $[x_i, x_{i+1}]$ for $i = k_n \ldots, I-2$. The six coefficients of the polynomial are obtained from six equations: $P_{n,i}(x_i) = c_n^i$, $P_{n,i}(x_{i+1}) = c_n^{i+1}$, $P_{n,i}(x_i)' = \partial_h c_n^i$, $P_{n,i}(x_{i+1})' = \partial_h c_n^{i+1}$, $P_{n,i}(x_i)'' = \partial_{hh} c_n^i$, $P_{n,i}(x_{i+1})'' = \partial_{hh} c_n^{i+1}$. On the segments $[x_{I-1}, x_I]$ we have only four equations because $\partial_h c_n^I$ and $\partial_{hh} c_n^I$ are not defined. Let us add the equations $P_{n,I-1}(x_I)' = \partial_h c_n^{I-1}$ and $P_{n,I-1}(x_I)'' = 0$. The equations for the coefficients are linear with a regular matrix (its determinant can be easily calculated). Finally we define $\psi_h(t, x)$ being linear with respect to t for $t \in [t_n, t_{n+1}]$, $x \in [x_i, x_{i+1}]$,

$$\psi_h(t, x) = P_{n,i}(x) + \frac{t - t_n}{\tau_n} \cdot \big(P_{n+1,i}(x) - P_{n,i}(x)\big).$$

Obviously $\partial_x\psi_h(t,x)$ and $\partial_{xx}\psi_h(t,x)$ are continuous and uniformly bounded, and $\partial_t\psi_h(t,x)$ and $\partial_{xt}\psi_h(t,x)$ exist between the nodes and are also uniformly bounded (see Theorems 3.6 and 3.7 and Corollary 3.8); thus

$$\psi_h(t_n+dt,x_i+dx)=\psi_h(t,x)+o(dt)+o(dx),$$
$$\partial_x\psi_h(t_n+dt,x_i+dx)=\partial_x\psi_h(t,x)+o(dt)+o(dx).$$

Due to the fact that $\psi_h(t,x)$, $\partial_x\psi_h(t,x)$, $\partial_t\psi_h(t,x)$, and $\partial_{xx}\psi_h(t,x)$ are uniformly bounded at the nodes, the functions $\psi_h(t,x)$ and $\partial_x\psi_h(t,x)$ are uniformly bounded and equicontinuous (even equi-Lipschitz) in $\aleph$.

Now take the sequence $h_j\to 0$ chosen above and consider the corresponding sequence $\psi_{h_j}(t,x)$. These functions are uniformly bounded and equicontinuous; by the Arzela–Ascoli theorem a uniformly convergent subsequence can be chosen. Let its limit be $\psi(t,x)$. It is continuous. Denote the corresponding subsequence of h_j again by h_j. It is clear that $\psi(t,x)\geq 1$, is bounded, and satisfies (1.5). Moreover, the derivatives $\partial_x\psi_h(t,x)$ are themselves uniformly bounded and equicontinuous. Applying the Arzela–Ascoli theorem, we learn that continuous $\partial_x\psi(t,x)$ exists and term-by-term differentiation is allowed.

PROPOSITION 7.1. *The function $\psi(t,x)$ is Lipschitz continuous in $\aleph$.*

Proof. Let $\vec{z}=(t,x)$ and bound

$$\begin{aligned}|\psi(\vec{z}_1)-\psi(\vec{z}_2)|&\leq|\psi(\vec{z}_1)-\psi_{h_j}(\vec{z}_1)|+|\psi_{h_j}(\vec{z}_1)-\psi_{h_j}(\vec{z}_2)|++|\psi(\vec{z}_2)-\psi_{h_j}(\vec{z}_2)|\\&\leq\varepsilon+Z'\|\vec{z}\|+\varepsilon=Z'\|\vec{z}\|+2\varepsilon.\end{aligned}$$

Here $\varepsilon>0$ is any number. We have used Lipschitz continuity of $\psi_{h_j}(\vec{z}_1)$ and their uniform convergence (assuming that j is large enough). Passing to the limit as $\varepsilon\to 0$ finishes the proof. ∎

THEOREM 7.2. *The free boundary $\rho(t)$ has negative Lipschitz continuous derivative for $t\in[0,T]$ and the Stefan condition (1.4) holds.*

Proof. Rewrite the Stefan condition (1.4) in integral form,

$$\rho(t)=\rho_0-\int_0^t\frac{g\big(c(\xi,\rho(\xi))\big)}{c\big(\xi,\rho(\xi)\big)}d\xi. \tag{7.1}$$

Substitute the approximations $\psi_h(t,x)$ and $\rho_h(t)$ into (7.1),

$$\rho_h(t)=\rho_0-\int_0^t\frac{g\big(\psi_h(t,\rho_h(t))\big)}{\psi_h(t,\rho_h(t))}d\xi+\Psi_h. \tag{7.2}$$

Here Ψ_h is the discrepancy. We need to prove that $\Psi_h\to 0$ as $h\to 0$.

First, let us study $\rho_h(t)$. Let $t_n\leq t\leq t_{n+1}$. We defined $\rho_h(t_n)$ by linear interpolation, so that

$$\rho_h(t_n)=\rho_0+\sum_{m=1}^{n}\partial_\tau\rho_m\tau_{m-1}.$$

Let μ_n be the set of natural $m\leq n$, such that $c_m^{k_m}$ is not small, i.e., $g\big(c_m^{k_m}\big)\geq\varphi'(\rho_0)\sqrt{h}$. Let $\bar{\mu}_n$ be its complement, i.e., $m=1,\dots,n$ that are not in μ_n. Now apply (6.1),

$$\begin{aligned}-\big(\rho_h(t_n)-\rho_0\big)&=-\sum_{m\in\mu_n}\partial_\tau\rho_m\tau_{m-1}=\sum_{m\in\mu_n}\frac{g\big(c_m^{k_m}\big)}{c_m^{k_m}}\tau_{m-1}\\&=\sum_{m=1}^{n}\frac{g\big(c_m^{k_m}\big)}{c_m^{k_m}}\tau_{m-1}-\sum_{m\in\bar{\mu}_n}\frac{g\big(c_m^{k_m}\big)}{c_m^{k_m}}\tau_{m-1}=\sum_{m=1}^{n}\frac{g\big(c_m^{k_m}\big)}{c_m^{k_m}}\tau_{m-1}+O\big(\sqrt{h}\big).\end{aligned}$$

The sum over $m \in \bar{\mu}_n$ has positive terms and each is at most $\varphi'(\rho_0)\sqrt{h}$; thus the sum is $O\big(\sqrt{h}\big)$. Note that $\rho_h(t) = \rho_h(t_n) + O(\tau_n) = \rho_h(t_n) + O\big(\sqrt{h}\big)$.

Let us consider

$$\int_0^{t_n} \frac{g\big(\psi_h(t,\rho_h(t))\big)}{\psi_h(t,\rho_h(t))} d\xi = \sum_{m=1}^{n} \int_{t_{m-1}}^{t_m} \frac{g\big(\psi_h(t,\rho_h(t))\big)}{\psi_h(t,\rho_h(t))} d\xi.$$

We have the continuous functions under the integrals; so that

$$\int_{t_{m-1}}^{t_m} \frac{g\big(\psi_h(t,\rho_h(t))\big)}{\psi_h(t,\rho_h(t))} d\xi = \frac{g\big(c_m^{k_m}\big)}{c_m^{k_m}}\tau_{m-1} + o(\tau_{m-1}) = \frac{g\big(c_m^{k_m}\big)}{c_m^{k_m}}\tau_{m-1} + o(\tau_{m-1}).$$

Let us rewrite $o(\tau_{m-1}) = \tau_{m-1}\omega_{m-1}$, $\omega_m \to 0$ as $h \to 0$. Then

$$\int_0^{t_n} \frac{g\big(\psi_h(t,\rho_h(t))\big)}{\psi_h(t,\rho_h(t))} d\xi = \sum_{m=1}^{n} \left(\frac{g\big(c_m^{k_m}\big)}{c_m^{k_m}}\right)\tau_{m-1} + \sum_{m=1}^{n} \omega_{m-1}\tau_{m-1}.$$

The last sum tends to zero as $h \to 0$; denote it by W. Note that

$$\int_0^{t} \frac{g\big(\psi_h(t,\rho_h(t))\big)}{\psi_h(t,\rho_h(t))} d\xi = \int_0^{t_n} \frac{g\big(\psi_h(t,\rho_h(t))\big)}{\psi_h(t,\rho_h(t))} d\xi + O(\tau_n).$$

Let us substitute the obtained expressions into (7.2),

$$O\big(\sqrt{h}\big) = O\big(\sqrt{h}\big) + W + \Psi_h.$$

Thus $\Psi_h \to 0$ as $h \to 0$ and the uniform limit of (7.2) exists. Therefore, the obtained continuous solution $\rho(t)$, $\psi(t,x)$ satisfies the integral Stefan equation (7.1). Its left-hand side $\rho(t)$ is not only continuous, but also has the continuous derivative for $t \in (0,T)$. Differentiating by t we see that the solution $\rho(t)$, $\psi(t,x)$ also satisfies the original Stefan condition (1.4). Moreover, the derivative $\dot\rho$ is Lipschitz because ψ is and $\dot\rho = g(\psi)/\psi$, where the right-hand side is smooth. ∎

COROLLARY 7.3. *The free boundary $\rho(t)$ has the inverse function $\rho^{-1}(x)$.*

8. Weak solution to the Dirichlet boundary-value problem. Let the set $Y_\rho(T) \subset \mathbb{R}^2$ contain all (t,x) such that $t \in (0,T)$, $x \in (\rho(t),L)$, let $\bar{Y}_\rho(T)$ be its closure. We are going to prove that $\psi(t,x)$ is the weak solution to problem (1.1)–(1.5) in $Y_\rho(T)$.

Consider the Dirichlet boundary-value problem,

$$\partial_t c(t,x) = \partial_{xx} c(t,x), \quad (t,x) \in Y_\rho(T), \tag{8.1}$$
$$c(t,L) = \psi(t,L), \quad c\big(t,\rho(t)\big) = \psi\big(t,\rho(t)\big), \quad t \in [0,T], \tag{8.2}$$
$$c(0,x) = \varphi(x), \quad x \in [\rho_0, L], \quad 0 < \rho_0 < L. \tag{8.3}$$

We are going to define a weak solution to this problem (similar to [7, 9, 10]).

DEFINITION 8.1. *A weak solution of the problem is a continuous function $c(t,x)$ that has the weak derivative $\partial_x c$ in $\bar{Y}_\rho(T)$ and satisfies conditions (8.2) and (8.3) and the integral identity*

$$\int_{\bar{Y}_\rho(T)} c(t,x)\partial_t v(t,x) dt dx = \int_{\bar{Y}_\rho(T)} \partial_x c(t,x)\partial_x v(t,x) dt dx$$

for each continuous in $\bar{Y}_\rho(T)$ function $v(t,x)$ with the weak derivative $\partial_x v$; the function v is such that $v(0,x) = v(T,x) = 0$, $v\big(t,\rho(t)\big) = v(t,L) = 0$.

Let us prove that the constructed function ψ is the only weak solution.

PROPOSITION 8.2. *The constructed solution $\psi(t,x)$ to the problem (1.1)–(1.5) is a weak solution to the problem (8.1)–(8.3).*

Proof. Boundary and initial conditions (8.2) and (8.3) are obviously satisfied. The identity is proved by considering it for the ψ_h up to the small errors and passing to the limit. ☐

THEOREM 8.3. *The weak solution to (8.1)–(8.3) is unique.*

Proof. Suppose [10] that there are two solutions $c_1(t,x)$ and $c_2(t,x)$; their difference $u(t,x) = c_1 - c_2$ also satisfies the identity; besides it satisfies the homogenous boundary conditions: $u(0,x) = 0$, $u\big(t,\rho(t)\big) = u(t,L) = 0$. Consider the function $v(t,x)$ such that $v(T,x) = 0$, $\partial_t v(t,x) = -u(t,x)$. Substitute $v(t,x)$ into the identity,

$$-\int_{\bar{Y}_\rho(T)} u^2 dtdx = \int_{\bar{Y}_\rho(T)} \partial_x u \int_t^T \partial_x u d\xi dtdx.$$

Let us transform the right-hand side,

$$\begin{aligned}\int\limits_{\bar{Y}_\rho(T)} \partial_x u \int\limits_t^T \partial_x u d\xi dtdx &= \int\limits_0^{\rho_0} \int\limits_{\rho^{-1}(x)}^T \partial_x u \int\limits_t^T \partial_x u d\xi dtdx + \int\limits_{\rho_0}^L \int\limits_0^T \partial_x u \int\limits_t^T \partial_x u d\xi dtdx \\ &= \int\limits_0^{\rho_0} \int\limits_{\rho^{-1}(x)}^T \partial_x u \int\limits_{\rho^{-1}(x)}^t \partial_x u d\xi dtdx + \int\limits_{\rho_0}^L \int\limits_0^T \partial_x u \int\limits_0^t \partial_x u d\xi dtdx.\end{aligned}$$

Adding the identities with these two forms on the right-hand side, we get

$$-2 \int\limits_{\bar{Y}_\rho(T)} u^2 dtdx = \int_0^{\rho_0} \int_{\rho^{-1}(x)}^T \partial_x u \int_{\rho^{-1}(x)}^T \partial_x u d\xi dtdx + \int_{\rho_0}^L \int_0^T \partial_x u \int_0^T \partial_x u d\xi dtdx.$$

The two integrals with ξ as the integration variable are independent of t. Thus,

$$-2 \int_{\bar{Y}_\rho(T)} u^2 dtdx = \int_0^{\rho_0} \left(\int_{\rho^{-1}(x)}^T \partial_x u dt \right)^2 dx + \int_{\rho_0}^L \left(\int_0^T \partial_x u dt \right)^2 dx.$$

This can hold only if $u \equiv 0$ in $\bar{Y}_\rho(T)$ and so the uniqueness is proved. ☐

As the solution to (8.1)–(8.3) is unique, there are no other solutions beside the function $\psi(t,x)$ constructed above .

9. Regularity. Let us show that the constructed solution $\psi(t,x)$ is actually classical, i.e., smooth, by applying results from [11]. First, we transform the domain to a rectangle by changing the spatial variable x in (8.1)–(8.3) in the following way: $x = \rho(t) + y \cdot \big(L - \rho(t)\big)$, $u(t,y) = c(t,x)$, $y \in [0,1]$, ρ is the obtained free boundary. The problem in the new variables looks like

$$\partial_t u(t,y) = a(t,y)\partial_{yy} u(t,y) + b(t,y)\partial_y u(t,y), \quad (t,y) \in D, \tag{9.1}$$

$$u(t,y) = \psi(t,y), \quad (t,y) \in \bar{B} \times S, \tag{9.2}$$

where $a = (L-\rho)^{-2}$, $b = (1-y)(L-\rho)^{-1}\dot{\rho}$, $D = \bar{B} \times [0,T]$ is a cylinder, $B = (0,1)$, $\bar{B} = [0,1]$, the boundary ∂B of B consists of two points, $x = 0$ and $x = 1$, and the boundary manifold S consists of two parts, $S_0 = (0,T) \times \{x = 0\}$ and $S_1 = (0,T) \times \{x = 1\}$. The

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function ψ is continuous in $\bar{Y}_\rho(T)$ and thus on $\bar{B} \times S$ also. Note that a does not depend on y. The notation is from [11].

Let us check the requirements of [11, Corollary 2, §4, Chapter III]. Condition $\bar{A}$ from [11] holds: the coefficients a, b are uniformly Hölder continuous in D; indeed, even Lipschitz continuous with the same Lipschitz constant. This follows from the fact that $\dot{\rho}$ is Lipschitz continuous. Condition B from [11] holds trivially: $a(t, y) \geq L^{-2} > 0$. The other requirements of [11] also hold trivially.

From [11, Corollary 2, §4, Chapter III], the existence of the unique classical solution u to the boundary-value problem (9.1)–(9.2) follows. The inverse change of variables $c(t, x) = u(t, y(x))$ provides us the classical solution of the problem (8.1)–(8.3) in $\bar{Y}_\rho(T)$. Being a classical solution, $c(t, x)$ is then a weak solution and thus coincides with the weak solution $\psi(t, x)$ (because the weak solution is unique). We have proved that $\psi(t, x)$ satisfies the boundary Stefan condition (1.4). The boundary conditions (1.2) and (1.3) also hold; the reason is that they obviously hold at the nodes of the lattice and the approximations have continuous derivatives with respect to x. Thus between the nodes the boundary conditions hold up to the error $O(\sqrt{dx^2 + dt^2})$, where $\sqrt{dx^2 + dt^2}$ is the distance to the nearest boundary node. Passing to the uniform limit as $h \to 0$ finishes the proof. Therefore, we have proven the following theorem.

THEOREM 9.1. *The constructed pair of the functions $\rho(t)$, $\psi(t, x)$ is the classical solution to the problem (1.1)–(1.5).*

The presented numerical method (algorithm) converges to a solution of the boundary-value problem (1.1)–(1.5) and can be used for solving the problem.

10. Numerical example. We illustrate the suggested method by a numerical example. The model is similar to that of [1]. Assume that the right-hand sides of the boundary conditions (1.2), (1.3), and the initial condition (1.5) are

$$G(c) = P - \beta c^2, \quad g(c) = \kappa c(c - 1), \quad \varphi(x) = \gamma_1 x + \gamma_2.$$

Here P is the sorption flux density, which is constant provided that the temperature and the pressure are constant; the desorption flux density βc^2 depends on the concentration c, the square law follows from the fact that two hydrogen atoms form a molecule H_2, $\beta < P$ is the desorption constant. The difference between sorption and desorption is the diffusion flux density, i.e., the right-hand side of (1.2). Hydride formation is described by the second formula, κ is constant (this boundary condition differs from the appropriate one from [1], where we assumed $c(t, \rho) = 1$). The initial distribution $\varphi(x)$ is stationary for the diffusion equation, i.e., is its time-independent solution. The constants γ_i are uniquely determined from the boundary conditions.

All assumptions hold, only $g'(c)$ is negative for $c < 0.5$. But this in not important because we have proved that $c \geq 1$, so we can change the condition for $c < 1$ without any influence on the results. After the time T, i.e., when hydriding is over, we have the problem of saturation with fixed boundaries and nonlinear boundary condition (1.2). Another condition follows from the symmetry and looks like $\partial_x c(t, 0) = 0$, thus $g(c) = 0$. All our results hold for this problem also. The dimensionless parameters were $L = 1$, $\rho_0 = 0.63$, $P = 1.21 \cdot 10^5$, $\beta = 1.24 \cdot 10^4$, $\kappa = 50$. To return to usual units it is enough to know $L = 7 \cdot 10^{-5}$ cm, the stoichiometric concentration in uranium $8.29 \cdot 10^{22}$ atoms per cm^3, and the hydrogen diffusivity in UH_3 $d = 7 \cdot 10^{-13}$ cm^2/s. The figures are in the usual units.

Figure 10.1 shows the flux densities at the boundaries; the upper curve is the flux density at $x = L$, the other is the flux density at the free boundary. It vanishes instantly when hydriding is over. Figure 10.2 displays the concentration at the free boundary; one can see that the assumption from [1] (that $c(t, \rho) \approx \mathrm{const}$ while hydriding is not over) is reasonable.

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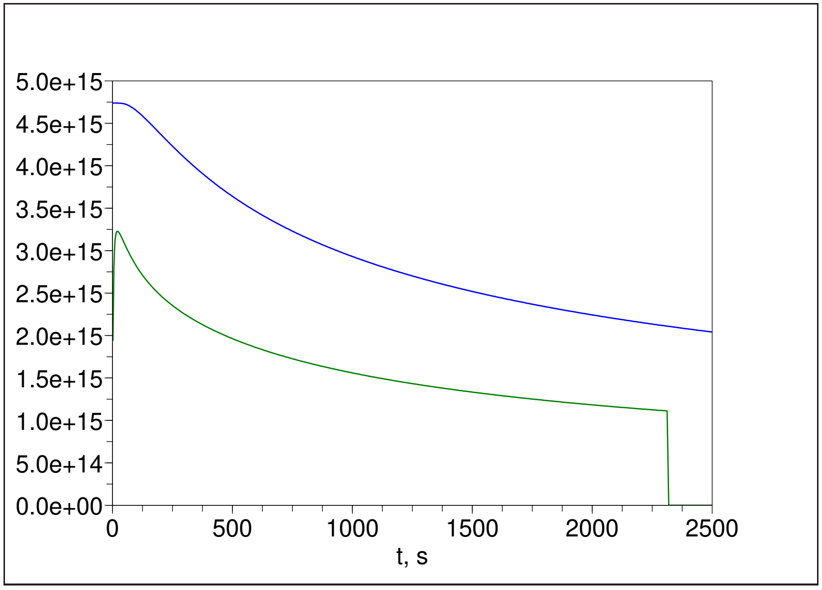

FIG. 10.1. *Flux densities at the boundaries.*

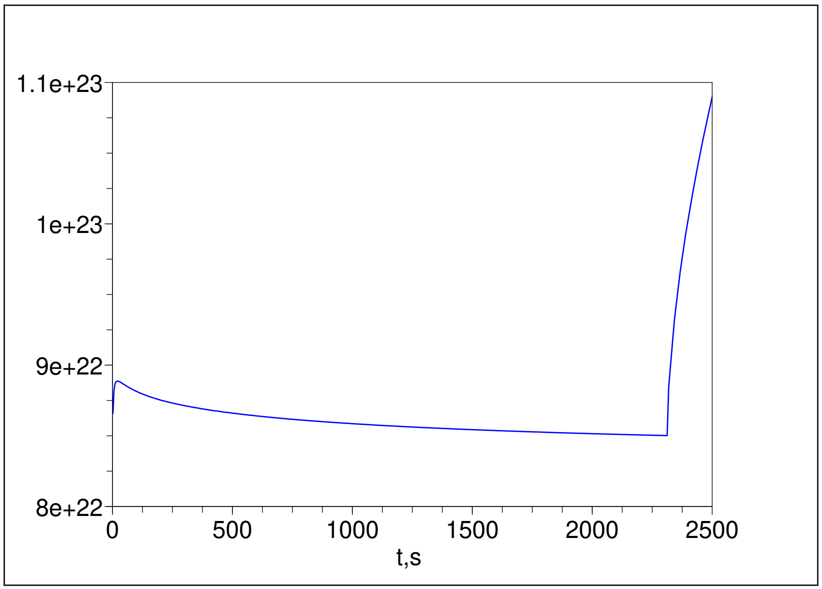

FIG. 10.2. *Concentration at the free boundary.*

In Figure 10.3 we present the concentration profiles at regularly distributed time instants. One can estimate the free boundary's velocity: it is almost constant. Also the concentration at $x = L$ is almost constant. This is the reason why we did not present it in Figure 10.2.

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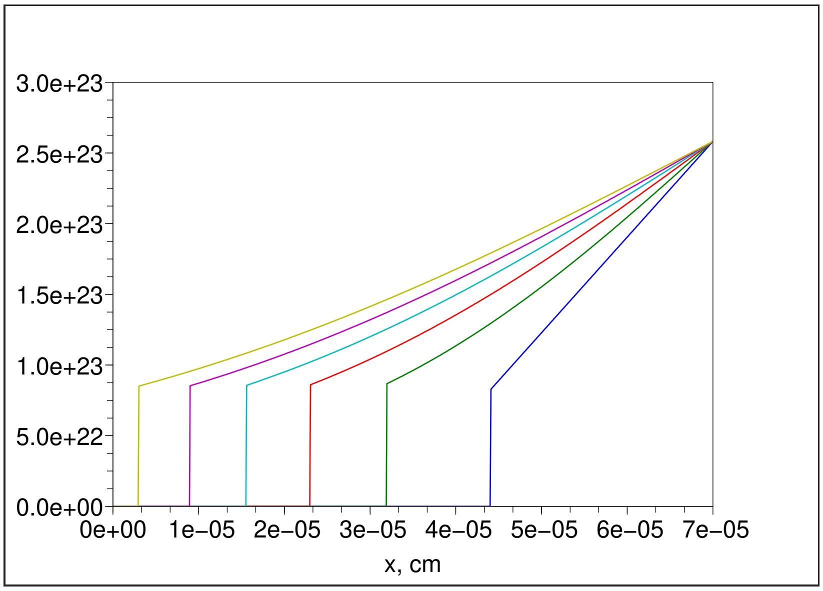

FIG. 10.3. *Concentration profiles.*

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