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Computing positive stable numerical solutions of moving boundary problems for concrete carbonation

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ABSTRACT

This paper deals with the construction and computation of numerical solutions of a coupled mixed partial differential equation system arising in concrete carbonation problems. The moving boundary problem under study is firstly transformed in a fixed boundary one, allowing the computation of the propagation front as a new unknown that can be computed together with the mass concentrations of CO_2 in air and water. Apart from the stability and the consistency of the numerical solution, constructed by a finite difference scheme, qualitative properties of the numerical solution are established. In fact, positivity of the concentrations, increasing properties of the propagation front and monotone behavior of the solution are proved. We also confirm numerically the $\sqrt{t}$-law of propagation. Results are illustrated with numerical examples.

1. Introduction

Environmental impact on concrete parts of buildings and civil engineering works such as bridges, sewage pipes and seawalls results in a variety of chemical and mechanical changes. The bulk of these changes leads to damaging and destabilization of the concrete itself or of the reinforcement embedded in the concrete. It is well known that in all carbonation scenarios, gaseous carbon dioxide is assumed to be supplied from an inexhaustible exterior source to the concrete sample, [1,2]. Carbon dioxide entering the non-saturated concrete sample through the air parts of the pores dissolves into the pore water and forms carbonic acid. This phenomenon, called concrete carbonation, may reduce the durability of reinforced concrete structures, causing the corrosion of the steel bars. The concrete carbonation level is measured throughout the CO_2 mass concentration in air and water phases in the concrete pores, that needs to be calculated. Gradually the process penetrates deeper into de concrete shaping a carbonation front that separates the carbonated zone from the uncarbonated one. A good understanding of the evolution of the carbonation process is crucial to predict the life service of concrete structures and save important amounts of money and energy.

Empirical evidences of the behavior of the carbonation front propagation have shown a dependence on time following the so-called $\sqrt{t}$-law, [3–10]. In the framework of moving-boundary problems, to our knowledge, Tuutti [11] in 1982, was the first appealing to the square root of t-law in the problem of concrete carbonation. Such conclusions were based on the Neumann solution of the two-phase Stefan problem, see Section 13.2.2 of [12].

In recent papers [1,13], the authors studied a one-dimensional free boundary problem modeling the carbonation process. The unknown CO_2 mass concentrations in air and water phases of pores are denoted by $U(t,x)$ and $V(t,x)$ respectively, depending on variables time t and space x. The space variable x is measured from the exposed boundary $x = 0$ to the

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unknown carbonation front $x = S(t)$. In the system (2)–(9) it is assumed that κ_1 and κ_2 are positive diffusion constants ($\kappa_1 \gg \kappa_2$) and the functions $f(U, V)$ and $\psi(r)$ are defined as

$$f(U, V) = \beta(\gamma V - U), \quad \beta > 0,\ \gamma > 0. \tag{1}$$

The continuous model is described by

$$\frac{\partial U}{\partial t} - \frac{\partial}{\partial x}\left(\kappa_1 \frac{\partial U}{\partial x}\right) = f(U, V), \quad 0 < t < T,\ 0 < x < S(t), \tag{2}$$

$$\frac{\partial V}{\partial t} - \frac{\partial}{\partial x}\left(\kappa_2 \frac{\partial V}{\partial x}\right) = -f(U, V), \quad 0 < t < T,\ 0 < x < S(t), \tag{3}$$

together with the left boundary conditions

$$U(t, 0) = G(t), \qquad V(t, 0) = H(t), \quad 0 \le t \le T. \tag{4}$$

The propagation front behavior comes out from the Stefan-like conditions, involving function $\psi(r)$ linked to the chemical reactions:

$$S'(t) = \psi(U(t, S(t))), \quad 0 < t < T, \tag{5}$$

$$-\kappa_1 \frac{\partial U}{\partial x}(t, S(t)) = \psi(U(t, S(t))) + S'(t)U(t, S(t)), \quad 0 < t < T, \tag{6}$$

$$-\kappa_2 \frac{\partial V}{\partial x}(t, S(t)) = S'(t)V(t, S(t)), \quad 0 < t < T. \tag{7}$$

Function $\psi(r)$ is given by

$$\psi(r) = \alpha|r|^p, \quad r \in \mathbb{R},\ \alpha > 0,\ p \ge 1, \tag{8}$$

where p is the so called order of the chemical reaction.

The bounded initial conditions functions are described by

$$S(0) = S_0, \qquad U(0, x) = U_0(x), \qquad V(0, x) = V_0(x), \quad 0 < x < S_0. \tag{9}$$

Aiki and Muntean [1,13] show qualitative properties of the solutions $U(t, x)$ and $V(t, x)$ of (2)–(9) as positivity and boundedness for fairly well posed initial conditions. Furthermore, they also justify rigorously that the carbonation front $S(t)$ satisfies a long time behavior of the type $C_1\sqrt{t} \le S(t) \le C_2\sqrt{t}$, when the exposed boundary conditions are constant, $G(t) = G^*$, $H(t) = H^*$, and linked by the condition $G^* = \gamma H^*$. Numerical simulations of the solution of carbonation problems using the finite element method have been performed in [14,15].

As the exact solution of the model (2)–(9) is not available and the best model may be wasted with a bad numerical analysis, in this paper we provide conditionally stable positive numerical solutions, apart from preserving the qualitative properties of the theoretical solution.

In Section 2, after a front-fixing transformation approach, the original problem is transformed into another one where the moving boundary becomes a new unknown of the problem, allowing the possibility to compute the expanding front. We propose a coupled finite difference scheme whose unknowns are both CO_2 concentrations, in air and water phases of pores, as well as the square power values of the expanding front. In Section 3, stability and positivity of the numerical solution is treated. The monotone increase in time behavior of the expanding front is shown numerically. We also prove for a fixed time the CO_2 concentrations are spatially decreasing from the exposed front to the carbonation front. Section 4 deals with a numerical conformation of the $\sqrt{t}$-law assumption. Numerical experiments illustrating the shown properties are included in the corresponding sections. Consistency of the proposed numerical scheme with the PDE problem is addressed in Section 5.

2. Front-fixing transformation and discretization

Let us begin this section by transforming the moving boundary problem (2)–(9) into another one with fixed boundary conditions. The Landau transformation, [16,17], suggests the substitution

$$L(t) = S^2(t), \qquad z(t, x) = \frac{x}{\sqrt{L(t)}}, \quad 0 \le t \le T,\ 0 < x < \sqrt{L(t)}. \tag{10}$$

Using substitution (10), the problem (2)–(9) becomes

$$L(t)\frac{\partial W}{\partial t} - L'(t)\frac{z}{2}\frac{\partial W}{\partial z} - \kappa_1 \frac{\partial^2 W}{\partial z^2} = L(t)\beta(\gamma Y - W), \quad 0 < t < T,\ 0 < z < 1, \tag{11}$$

$$L(t)\frac{\partial Y}{\partial t} - L'(t)\frac{z}{2}\frac{\partial Y}{\partial z} - \kappa_2 \frac{\partial^2 Y}{\partial z^2} = -L(t)\beta(\gamma Y - W), \quad 0 < t < T,\ 0 < z < 1, \tag{12}$$

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where

$$W(t,z) = U(t,x), \qquad Y(t,z) = V(t,x). \tag{13}$$

In addition, the new boundary conditions take the form

$$W(t,0) = G(t), \qquad Y(t,0) = H(t), \quad 0 \le t \le T. \tag{14}$$

The Stefan-like conditions (5)–(7) are transformed into

$$L'(t) = 2\sqrt{L(t)}\alpha[W(t,1)]^p, \quad 0 < t < T, \tag{15}$$

$$-2\kappa_1 \frac{\partial W}{\partial z}(t,1) = L'(t)(1 + W(t,1)), \quad 0 < t < T, \tag{16}$$

$$-2\kappa_2 \frac{\partial Y}{\partial z}(t,1) = L'(t)Y(t,1), \quad 0 < t < T, \tag{17}$$

and the initial conditions (9) become

$$L(0) = L_0; \qquad W(0,z) = W_0(z) = U_0(zS_0); \qquad Y(0,z) = Y_0(z) = V_0(zS_0), \quad 0 < z < 1. \tag{18}$$

Note that the transformed problem (11)–(18) is an initial-fixed boundary problem for a system of two nonlinear parabolic partial differential equations in the bounded fixed domain $(0,T) \times (0,1)$.

Let N and M be positive integers and let us consider the step sizes discretizations $k = \Delta t = T/N$, $h = \Delta z = 1/M$ and the mesh points (t^n, z_j), with $t^n = nk$, $z_j = jh$, $0 \le n \le N$, $0 \le j \le M$. Numerical approximations of the involved variables are denoted by: $w_j^n \approx W(t^n, z_j)$, $y_j^n \approx Y(t^n, z_j)$, $l^n \approx L(t^n)$, while we denote $G^n = G(t^n)$, $H^n = H(t^n)$.

Partial derivatives at the interior points are approximated using forward in time and centered in space finite difference expressions:

$$\frac{w_j^{n+1} - w_j^n}{k} \approx \frac{\partial W}{\partial t}(t^n, z_j), \qquad \frac{y_j^{n+1} - y_j^n}{k} \approx \frac{\partial Y}{\partial t}(t^n, z_j), \qquad \frac{l^{n+1} - l^n}{k} \approx L'(t^n), \tag{19}$$

$$\frac{w_{j+1}^n - w_{j-1}^n}{2h} \approx \frac{\partial W}{\partial z}(t^n, z_j), \qquad \frac{w_{j-1}^n - 2w_j^n + w_{j+1}^n}{h^2} \approx \frac{\partial^2 W}{\partial z^2}(t^n, z_j), \tag{20}$$

$$\frac{y_{j+1}^n - y_{j-1}^n}{2h} \approx \frac{\partial Y}{\partial z}(t^n, z_j), \qquad \frac{y_{j-1}^n - 2y_j^n + y_{j+1}^n}{h^2} \approx \frac{\partial^2 Y}{\partial z^2}(t^n, z_j). \tag{21}$$

To preserve the second order accuracy at the right boundary $z = 1$, we take left side approximations with three points:

$$\frac{3w_M^n - 4w_{M-1}^n + w_{M-2}^n}{2h} \approx \frac{\partial W}{\partial z}(t^n, 1), \qquad \frac{3y_M^n - 4y_{M-1}^n + y_{M-2}^n}{2h} \approx \frac{\partial Y}{\partial z}(t^n, 1). \tag{22}$$

Using the approximations (19)–(21), Eqs. (11)–(12) become discretized at the interior mesh points in the following way

$$l^n \frac{w_j^{n+1} - w_j^n}{k} - \frac{z_j}{2} \frac{w_{j+1}^n - w_{j-1}^n}{2h} \left(\frac{l^{n+1} - l^n}{k} \right) - \kappa_1 \frac{w_{j-1}^n - 2w_j^n + w_{j+1}^n}{h^2}$$
$$= l^n \beta(\gamma y_j^n - w_j^n), \quad 0 \le n \le N-1, \ 1 \le j \le M-1, \tag{23}$$

$$l^n \frac{y_j^{n+1} - y_j^n}{k} - \frac{z_j}{2} \frac{y_{j+1}^n - y_{j-1}^n}{2h} \left(\frac{l^{n+1} - l^n}{k} \right) - \kappa_2 \frac{y_{j-1}^n - 2y_j^n + y_{j+1}^n}{h^2}$$
$$= -l^n \beta(\gamma y_j^n - w_j^n), \quad 0 \le n \le N-1, \ 1 \le j \le M-1. \tag{24}$$

Initial conditions given in (18) take the discrete form

$$l^0 = S^2(0) = S_0^2, \qquad w_j^0 = U_0(z_j S_0), \qquad y_j^0 = V_0(z_j S_0), \quad 1 \le j \le M-1. \tag{25}$$

Note that the starting values w_M^0 and y_M^0 are not given and need to be obtained.

Left boundary conditions are discretized as

$$w_0^n = G^n, \qquad y_0^n = H^n, \quad 0 \le n \le N. \tag{26}$$

The discretization of the Stefan-like conditions (15)–(17) takes the form

$$\frac{l^{n+1} - l^n}{k} = 2\alpha (l^n)^{\frac{1}{2}} (w_M^n)^p, \quad 0 \le n \le N-1, \tag{27}$$

$$-\kappa_1 \frac{3w_M^n - 4w_{M-1}^n + w_{M-2}^n}{h} = \frac{l^{n+1} - l^n}{k}(1 + w_M^n), \quad 0 \le n \le N-1, \tag{28}$$

$$-\kappa_2 \frac{3y_M^n - 4y_{M-1}^n + y_{M-2}^n}{h} = \frac{l^{n+1} - l^n}{k} y_M^n, \quad 0 \le n \le N-1. \tag{29}$$

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For the sake of clarity we explain how to transit from the time level n to $n+1$. Firstly, solving (27)–(29) for $n=0$ one gets the starting unknown values w_M^0 and y_M^0, as well as l^1. Then, from the values for the time level n, $\{w_j^n, y_j^n, l^n;\ 0 \le j \le M-1\}$, one needs to obtain the remaining values $\{w_M^n, y_M^n\}$ and $\{w_j^{n+1}, y_j^{n+1}, l^{n+1};\ 1 \le j \le M-1\}$. Note that the nonlinear system (27)–(28) is coupled in the unknowns w_M^n and l^{n+1}. From (27) one gets

$$l^{n+1} = l^n + 2k\alpha (l^n)^{\frac{1}{2}} (w_M^n)^p, \quad 0 \le n \le N-1. \tag{30}$$

By substituting (30) in (28) the following nonlinear equation in w_M^n for each step n must be solved

$$F_n(w_M^n) = 0, \quad 0 \le n \le N, \tag{31}$$

where $F_n : [0, \infty[\to \mathbb{R}$, is given by

$$F_n(\xi) = 2\alpha (l^n)^{\frac{1}{2}} \xi^{p+1} + 2\alpha (l^n)^{\frac{1}{2}} \xi^p + \frac{3\kappa_1}{h}\xi - \frac{\kappa_1}{h}(4w_{M-1}^n - w_{M-2}^n). \tag{32}$$

We solve Eqs. (31)–(32) using Newton iteration method. Once w_M^n is calculated solving (31)–(32), the unknown l^{n+1} is given by (30) and y_M^n is computed using (29). In this process, positivity of the involved quantities w_M^n, l^n and y_M^n has to be proved. This positiveness requirement is fulfilled in Section 3.

Finally, Eqs. (23)–(24) allow to obtain explicitly the solutions at the interior points at time level $n+1$ as follows

$$w_j^{n+1} = a_{1,j}^n w_{j-1}^n + b_{1,j}^n w_j^n + c_{1,j}^n w_{j+1}^n + k\beta\gamma y_j^n, \quad 0 \le n \le N-1,\ 1 \le j \le M-1, \tag{33}$$

$$y_j^{n+1} = a_{2,j}^n y_{j-1}^n + b_{2,j}^n y_j^n + c_{2,j}^n y_{j+1}^n + k\beta w_j^n, \quad 0 \le n \le N-1,\ 1 \le j \le M-1, \tag{34}$$

where

$$a_{i,j}^n = \frac{\kappa_i k}{h^2 l^n} - \frac{z_j}{4h}\Delta^n, \qquad c_{i,j}^n = \frac{\kappa_i k}{h^2 l^n} + \frac{z_j}{4h}\Delta^n, \quad i = 1, 2,$$
$$b_{1,j}^n = 1 - k\beta - \frac{2\kappa_1 k}{h^2 l^n}, \qquad b_{2,j}^n = 1 - k\beta\gamma - \frac{2\kappa_2 k}{h^2 l^n}, \tag{35}$$

and

$$\Delta^n = \frac{l^{n+1}}{l^n} - 1. \tag{36}$$

We summarize the construction of the numerical solution in the procedure exposed in Algorithm 1.

3. Positivity, stability and monotonicity of the numerical solution

Dealing with concentrations, the positivity of the computed values is not an alternative but a necessity that needs to be guaranteed. We use an inductive method where, under the assumption that values $\{w_j^n, y_j^n, l^n;\ 1 \le j \le M-1\}$ are positive, we show the positivity of the elements of $\{w_j^{n+1}, y_j^{n+1}, l^{n+1};\ 1 \le j \le M-1\}$, as well as the positivity of the remaining values on the right boundary of the discrete domain, $\{w_M^n, y_M^n\}$.

Let us start showing the positivity of the solution w_M^n of Eqs. (31)–(32) paying attention to the last term of Eq. (32). Note that from Taylor's theorem one has

$$w_{M-2}^n = w_{M-1}^n - h\frac{\partial W}{\partial z}(t^n, \xi); \quad (M-2)h < \xi < (M-1)h. \tag{37}$$

Let E_n be defined by

$$E_n = \max \left| \frac{\partial W}{\partial z}(t^n, z) \right|, \quad 0 \le z \le 1, \tag{38}$$

from (37) and (38)

$$|w_{M-2}^n - w_{M-1}^n| < E_n h. \tag{39}$$

Hence, taking $h < 3w_{M-1}/E_n$, one gets

$$4w_{M-1}^n - w_{M-2}^n = 3w_{M-1}^n + (w_{M-1}^n - w_{M-2}^n) > 3w_{M-2}^n - E_n h > 0. \tag{40}$$

Let us denote $\delta^n = (4w_{M-1}^n - w_{M-2}^n)/3 > 0$ and note that $F_n(\xi)$ defined by (32) is a continuous strictly increasing function satisfying $F_n(0) = (-3\kappa_1/h)\delta^n < 0$ and $F_n(\delta^n) > 0$, for each $n \ge 0$. Thus, there exists a unique point ξ_*^n such that $0 < \xi_*^n < \delta^n$ and $F_n(\xi_*^n) = 0$. This unique solution of (31)–(32) is the required value $w_M^n = \xi_*^n > 0$.

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Algorithm 1: Calculation procedure for (w_j^n, y_j^n, l^n)

Data: Initial conditions given in (25); Boundary conditions given in (26).
Result: Solution (w_j^n, y_j^n, l^n) of the problem (23)–(29).

```
n=0;
while n ≤ N do
    Compute w_M^n solving (31)–(32) by Newton–Raphson method:
    Data: (w_M^n)^0, Initial estimate of w_M^n; e, Tolerance.
    Result: w_M^n.
    i=0;
    (w_M^n)^1 = (w_M^n)^0 − F_n((w_M^n)^0)/F_n'((w_M^n)^0);
    while |((w_M^n)^{i+1} − (w_M^n)^i)/(w_M^n)^{i+1}| ≥ e do
        i=i+1;
        (w_M^n)^{i+1} = (w_M^n)^i − F_n((w_M^n)^i)/F_n'((w_M^n)^i);
    end
    Compute l^{n+1} by (30);
    Compute y_M^n using (29);
    while n ≤ N − 1 do
        for j = 1, ..., M − 1 do
            Obtain w_j^{n+1} by (33);
            Obtain y_j^{n+1} by (34);
        end
    end
    n=n+1;
end
```

From (30) and induction principle, it follows that

$$0 < l^n < l^{n+1}, \quad 0 \le n \le N-1. \tag{41}$$

From (29), one gets

$$y_M^n = k\left[\frac{\kappa_2(4y_{M-1}^n - y_{M-2}^n)}{3k\kappa_2 + h(l^{n+1} - l^n)}\right], \quad 0 \le n \le N-1. \tag{42}$$

Positivity of $(4y_{M-1}^n - y_{M-2}^n)$ for small enough values of h, is obtained in analogous way to the proof of the same result for $(4w_{M-1}^n - w_{M-2}^n)$. Using (41) and (42) we have that $y_M^n > 0$.

Regarding to the positivity of the remaining w_j^{n+1} and y_j^{n+1}, $1 \le j \le M-1$, let us study the nonnegativity of the coefficients (35) of the scheme (33)–(34). From (35) and (41) one gets that $c_{i,j}^n > 0$, $i = 1, 2$, and

$$b_{1,j}^n \ge 1 - k\beta - \frac{2\kappa_1 k}{h^2 l^0}, \qquad b_{2,j}^n \ge 1 - k\beta\gamma - \frac{2\kappa_2 k}{h^2 l^0}. \tag{43}$$

Then, coefficients $b_{i,j}^n$, $i = 1, 2$, are positive under the condition

$$k < k_0 = \min\{k_1, k_2\}, \tag{44}$$

where

$$k_1 = \frac{h^2 l_0}{2\kappa_1 + h^2\beta l_0}, \qquad k_2 = \frac{h^2 l_0}{2\kappa_2 + h^2\beta\gamma l_0}. \tag{45}$$

Now we address the nonnegativity of the coefficients $a_{1,j}^n$, whose sign depends on the difference $l^{n+1} - l^n$ and, from the discretization of the Stefan-like condition (28), this difference involves w_M and $(4w_{M-1} - w_{M-2})$.

In order to simplify these relationships, let us consider the right-hand side approximation of the spatial partial derivative of $W(t, z)$ at $(t^n, 1)$

$$\frac{-3w_M^n + 4w_{M+1}^n - w_{M+2}^n}{2h} = \frac{\partial W}{\partial z}(t^n, 1) + \mathcal{O}(h^2), \tag{46}$$

where the artificial values w_{M+1}^n and w_{M+2}^n vanish because they are outside of the real carbonated region.

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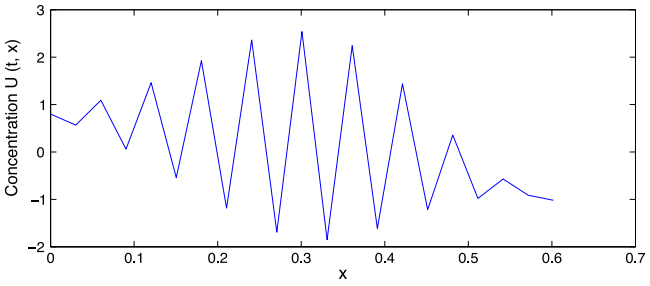

Fig. 1. Numerical solution of Example 1 for $t = 0.375$ years, when positivity condition is broken.

In agreement with (22), left-hand side backward approximation of the spatial partial derivative of $W(t, z)$ at $(t^n, 1)$ satisfies

$$\frac{3w_M^n - 4w_{M-1}^n + w_{M-2}^n}{2h} = \frac{\partial W}{\partial z}(t^n, 1) + \mathcal{O}(h^2). \tag{47}$$

From (46)–(47), one gets

$$6w_M^n = 4w_{M-1}^n - w_{M-2}^n + \mathcal{O}(h^3). \tag{48}$$

Using (28) and (48), it follows that

$$l^{n+1} - l^n = \frac{k\kappa_1}{h}\frac{3w_M^n}{1 + w_M^n} + \mathcal{O}(kh^2), \tag{49}$$

and from (35) and (49), using that $0 < z_j \leq 1$,

$$a_{1,j}^n \geq \frac{\kappa_1 k}{h^2 l^n}\left(\frac{4 + w_M^n}{4(1 + w_M^n)} + \mathcal{O}(h^3)\right). \tag{50}$$

Hence, for small enough values of k and h, coefficients $a_{1,j}^n$ are positive. Finally, from the expression (35) for $a_{2,j}^n$, managing the values of y_M^n and $(4y_{M-1}^n - y_{M-2}^n)$ in analogous way to the previous study with w_j^n, one gets

$$6y_M^n = 4y_{M-1}^n - y_{M-2}^n + \mathcal{O}(h^3), \tag{51}$$

$$l^{n+1} - l^n = \frac{3k\kappa_2}{h} + \mathcal{O}(kh^2), \tag{52}$$

and

$$a_{2,j}^n \geq \frac{\kappa_2 k}{h^2 l^n}\left(\frac{1}{4} + \mathcal{O}(h^3)\right). \tag{53}$$

Summarizing, the following result has been established:

Theorem 1. *With previous notation, for small enough values of the step sizes h and k linked by the condition (44)–(45), the following conclusions hold true:*

(i) *Concentration solutions of the scheme (33)–(34) w_j^n and y_j^n are positive for $1 \leq j \leq M - 1$, $1 \leq n \leq N$.*
(ii) *Concentrations at the right boundary w_M^n and y_M^n are positive.*
(iii) *The moving carbonation front is positive and increasing, $0 < l^0 < l^1 < \cdots < l^N$.*

The positivity guaranteed by Theorem 1 is not unconditional and the following example shows that this condition cannot be removed.

Example 1. In accordance with [15], consider the carbonation model (2)–(9) with parameters listed in Table 1 and time horizon $T = 15$ years. For $h = 0.05$, one gets $k_1 = 0.0062$ and $k_2 = 0.0625$. Taking $k = 0.0075$, the positivity condition is broken. Fig. 1 shows that positivity does not hold. Units in x-axes are taken in cm and y-axes in 10^{-6} g cm^{-3}.

Apart from the positivity of the numerical solution, a crucial requirement is the stability of such numerical solution. For the sake of clarity in the presentation and because of the existence in the literature of several definitions of stability, we precise the concept of stability we use. As the stability is related to the boundedness of the numerical solution, we need to precise a norm. We denote the so called supremum norm of a vector $x = (x_1, x_2, \ldots, x_n)^T$ in $\mathbb{R}^n$ as $\|x\|_\infty = \max(|x_1|, |x_2|, \ldots, |x_n|)$.

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Table 1
Data for numerical examples.

Magnitude	Value
Initial concentrations ($10^{-6} \times$ g cm^{-3})	
$U_0(x)$, $0 < x < S_0$	0.80–1.50x
$V_0(x)$, $0 < x < S_0$	200 000–398 000x
Exposed boundary concentrations ($10^{-6} \times$ g cm^{-3})	
$G(t)$	0.80
$H(t)$	200 000
Diffusion constants ($10^8 \times$ cm^2 year^{-1})	
κ_1	0.05
κ_2	0.005
Model parameters	
α	1.00
β (year^{-1})	0.001
γ	5×10^{-6}
p	2.00
Initial position of carbonation front (cm)	
S_0	0.50

Definition 1. With previous notation, let us denote the vectors of CO_2 concentrations $w^n = [w_0^n, w_1^n, \ldots, w_M^n]^T$ and $y^n = [y_0^n, y_1^n, \ldots, y_M^n]^T$. We say that the numerical solution $\{w^n, y^n,\ 0 \le n \le N\}$ is $\|\cdot\|_\infty$-stable if there exist positive constants C_1 and C_2 independent of n, k and h, such that

$$\|w^n\|_\infty \le C_1, \qquad \|y^n\|_\infty \le C_2, \quad 0 \le n \le N. \tag{54}$$

Now we show that under the positivity conditions of Theorem 1, the numerical solution $\{w_j^n, y_j^n\}$ is $\|\cdot\|_\infty$-stable. Let $G(t)$ and $H(t)$ be the left boundary conditions given by (4) and let $U_0(x)$ and $V_0(x)$ be the initial conditions given by (9). Let $\tilde{G}$ and $\tilde{H}$ be positive upper bounds such that

$$\left.\begin{array}{l} G(t) \le \tilde{G}, \qquad H(t) \le \tilde{H}, \quad 0 \le t \le T, \\ U_0(z_j S_0) = w_j^0 \le \tilde{G}, \qquad V_0(z_j S_0) = y_j^0 \le \tilde{H}, \quad 1 \le j \le M-1, \\ \tilde{G} = \gamma \tilde{H}. \end{array}\right\} \tag{55}$$

From (48) and (51) evaluated at $n = 0$ it follows

$$w_M^0 < \frac{2}{3} w_{M-1}^0 \le \tilde{G}, \qquad y_M^0 < \frac{2}{3} y_{M-1}^0 \le \tilde{H}. \tag{56}$$

Once we have the bound at the time level $n = 0$, we prove using the induction principle the boundedness of the numerical solution for all the time levels. Let us assume the induction hypothesis

$$w_j^n \le \tilde{G}, \qquad y_j^n \le \tilde{H}, \quad 1 \le j \le M, \ \tilde{G} = \gamma \tilde{H}. \tag{57}$$

From (33)–(34) and (35) under the conditions of Theorem 1 one gets, for $1 \le j \le M-1$,

$$w_j^{n+1} \le (a_{1,j}^n + b_{1,j}^n + c_{1,j}^n)\tilde{G} + k\beta\gamma\tilde{H} = (1 - k\beta)\tilde{G} + k\beta\gamma\tilde{G} = \tilde{G}, \tag{58}$$

$$y_j^{n+1} \le (a_{2,j}^n + b_{2,j}^n + c_{2,j}^n)\tilde{H} + k\beta\tilde{G} = (1 - k\beta\gamma)\tilde{H} + k\beta\tilde{G} = \tilde{H}. \tag{59}$$

Furthermore, using (48) and (51), together with (58)–(59) for $j = M-1$, it follows that $w_M^{n+1} \le \tilde{G}$ and $y_M^{n+1} \le \tilde{H}$.
Summarizing the following conditional stability result has been established:

Theorem 2. *With previous notation, for small enough values of h and k satisfying the positivity step size condition (44)–(45), the numerical solution of scheme (33)–(34) is $\|\cdot\|_\infty$-stable.*

As it has been shown in Example 1, where the positivity does not occur when the positivity condition (44)–(45) was broken, in the following example we show that when the positivity condition is satisfied, then we have both positivity and $\|\cdot\|_\infty$-stability.

Example 2. With the notation and the parameters of Example 1, and step sizes $h = 0.05$ and $k = 0.005$, the stability of the solutions $U(t, x)$ and $V(t, x)$ is guaranteed as it is shown in Fig. 2. Units in x-axes are taken in cm and y-axes in 10^{-6} g cm^{-3}.

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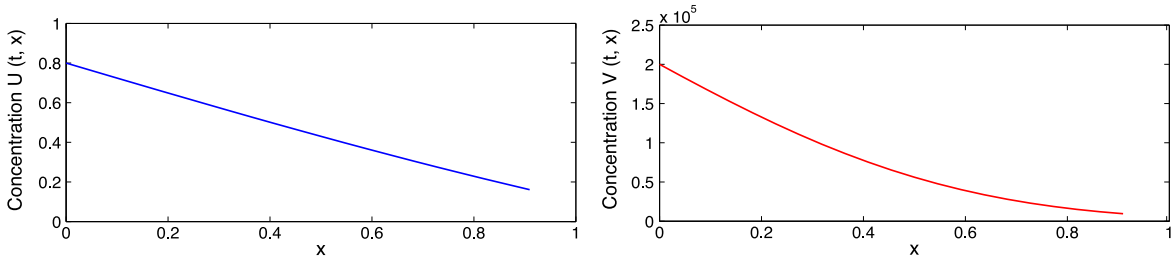

Fig. 2. Numerical solution of $U(t,x)$ and $V(t,x)$ in Example 2 for $t = 13$ years, under stability condition.

An important property of the numerical solution is its monotone decreasing behavior with respect to the space from the exposed boundary to the carbonation front at each time level under the positivity step size conditions. For the sake of clarity in the presentation and the concept of monotone schemes has been used earlier in the literature [18], we introduce the following definition:

Definition 2. With previous notation, we say that the numerical scheme (33)–(34) is spatial monotone preserving, if assuming that the numerical solution is spatial monotone decreasing at time level n, $0 \le n \le N-1$, i.e.,:

$$w_{j+1}^n \le w_j^n, \qquad y_{j+1}^n \le y_j^n, \quad 0 \le j \le M-1, \tag{60}$$

then, one satisfies

$$w_{j+1}^{n+1} \le w_j^{n+1}, \qquad y_{j+1}^{n+1} \le y_j^{n+1}, \quad 0 \le j \le M-1. \tag{61}$$

Now we state that, under the positivity constraints (44)–(45) on the coefficients (35) together with an additional condition for concentrations at the exposed boundary, the numerical scheme is spatial monotone preserving. This condition imposes that $G(t)$ and $H(t)$ are time monotone non decreasing functions satisfying

$$G(t) = \gamma H(t), \quad 0 \le t \le T. \tag{62}$$

From Eq. (33), the positivity of coefficients $a_{1,j}^n$, $b_{1,j}^n$, $c_{1,j}^n$ and the induction hypothesis of Definition 2, it follows that $w_{j-1}^n \ge w_j^n$, $w_j^n \ge w_{j+1}^n$,

$$\begin{aligned} w_j^{n+1} &\ge a_{1,j}^n w_j^n + b_{1,j}^n w_j^n + c_{1,j}^n w_j^n + k\beta\gamma y_j^n \\ &= \left(1 - k\beta - \frac{\kappa_1 k}{h^2 l^n} - \frac{j}{4}\Delta^n\right) w_j^n + c_{1,j}^n w_{j+1}^n + k\beta\gamma y_j^n, \quad 1 \le j \le M-1, \end{aligned} \tag{63}$$

and

$$\begin{aligned} w_{j+1}^{n+1} &\le a_{1,j+1}^n w_j^n + b_{1,j}^n w_{j+1}^n + c_{1,j+1}^n w_{j+1}^n + k\beta\gamma y_{j+1}^n \\ &= \left(1 - k\beta - \frac{\kappa_1 k}{h^2 l^n} + \frac{j+1}{4}\Delta^n\right) w_{j+1}^n + a_{1,j+1}^n w_j^n + k\beta\gamma y_j^n, \quad 1 \le j \le M-2. \end{aligned} \tag{64}$$

From (63) and (64) and the hypothesis condition of Definition 2 it follows that

$$w_{j+1}^{n+1} - w_j^{n+1} \le \left(b_{1,j}^n + \frac{1}{4}\Delta^n\right)(w_{j+1}^n - w_j^n) + k\beta\gamma(y_{j+1}^n - y_j^n) \le 0, \quad 1 \le j \le M-2. \tag{65}$$

Furthermore $w_M^{n+1} < w_{M-1}^{n+1}$ due to (56). Using Eq. (33) for $j = 1$, hypothesis of Definition 2 and assuming that $G(t)$ and $H(t)$ are monotone non decreasing functions satisfying (62), it follows

$$\begin{aligned} w_1^{n+1} &\le (a_{1,1}^n + b_{1,1}^n + c_{1,1}^n) w_0^n + k\beta\gamma y_0^n \\ &\le (1 - k\beta) G^n + k\beta\gamma H^n = G^n \le G^{n+1} = w_0^{n+1}. \end{aligned} \tag{66}$$

The monotonicity of $\{y_j^{n+1}\}$ can be shown in an analogous way to that used for $\{w_j^{n+1}\}$, and the following result has been established.

Theorem 3. *With previous notation, under the positivity conditions (44)–(45), assuming that the concentrations at the exposed boundary are monotone non decreasing functions such that $G(t) = \gamma H(t)$, then the numerical scheme (33)–(34) is spatial monotone preserving.*

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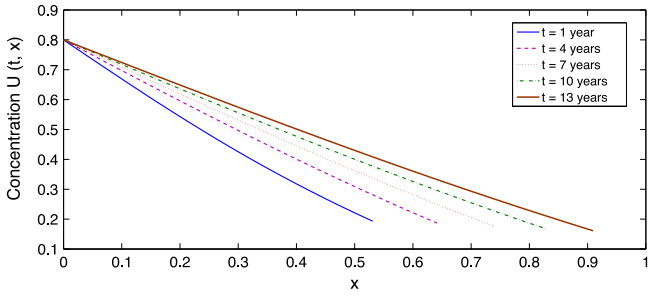

Fig. 3. Numerical solution $U(t, x)$ of Example 3 for several equidistant times t_i.

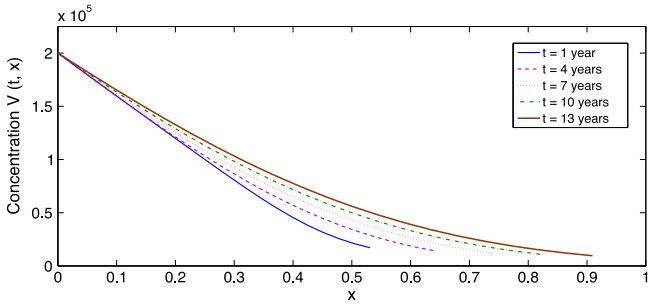

Fig. 4. Numerical solution $V(t, x)$ of Example 3 for several equidistant times t_i.

Table 2
Carbonation depth for several times.

t_i (years)	33.00	33.50	34.00	34.50	35.00
$S(t_i)$ (cm)	1.3407	1.3499	1.3591	1.3682	1.3772

Next Example 3 illustrates the decreasing monotonicity behavior of both concentrations $U(t, x)$ and $V(t, x)$ in the space variable when the time is fixed.

Example 3. With data of Table 1 and taking step sizes $h = 0.05$ and $k = 0.005$ satisfying the monotonicity requirements of Theorem 3, Figs. 3 and 4 show the monotone behavior of the functions $U(t_i, x)$ and $V(t_i, x)$ corresponding to the mass concentrations of CO_2 in air and water, respectively. Here t_i, $1 \leq i \leq 5$, represent four equidistant fixed values of time. Note also that the carbonation zone is increasing with time, according to the spreading of the propagation front $S(t)$, see Theorem 1(iii).

4. Numerical evidences of the $\sqrt{t}$-law of propagation

In this section we confirm numerically, under appropriated positivity conditions, that the proposed numerical solution behaves as the theoretical solution suggested. In fact, in the next example, according to data from [15], we match the numerical solution of the carbonation front as a function of the type $C\sqrt{t}$.

Example 4. With the same parameters and step size values of Example 2, Table 2 shows long time values of the carbonation front $S(t)$ on time, with a time horizon of $T = 35$ years. These points $(t_i, S(t_i))$ have been fitted to a curve with two parameters of the type $S(t) = at^b$. The best fit (in the least square sense) is matched by $a = 0.2715$ and $b = 0.4568$, and the coefficient of determination $R^2 = 0.9999$. This numerical experiment illustrates the agreement with the behavior of the theoretical solution.

5. Consistency

Consistency of a numerical scheme with a PDE problem means that the theoretical solution of the problem approximates well the numerical scheme when the step size discretizations tend to zero. So, a numerical scheme can be consistent with an equation and not with another one, see [19], Chap. 2, and [20], Chap. 1. Thus, it is important to address the consistency of a numerical scheme with a problem.

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Equations of the problem (11)–(17) can be written in vector form as $\mathcal{L}(W,Y,L) = (\mathcal{L}_1(W,Y,L), \mathcal{L}_2(W,Y,L), \mathcal{L}_3(W,L), \mathcal{L}_4(W,L), \mathcal{L}_5(Y,L)) = 0$, in which

$$\mathcal{L}_1(W,Y,L) = L(t)\frac{\partial W}{\partial t} - L'(t)\frac{z}{2}\frac{\partial W}{\partial z} - \kappa_1\frac{\partial^2 W}{\partial z^2} - L(t)\beta(\gamma Y - W) = 0, \quad t > 0,\ 0 < z < 1, \tag{67}$$

$$\mathcal{L}_2(W,Y,L) = L(t)\frac{\partial Y}{\partial t} - L'(t)\frac{z}{2}\frac{\partial Y}{\partial z} - \kappa_2\frac{\partial^2 Y}{\partial z^2} + L(t)\beta(\gamma Y - W) = 0, \quad t > 0,\ 0 < z < 1, \tag{68}$$

$$\mathcal{L}_3(W,L) = L'(t) - 2\big(L(t)\big)^{\frac{1}{2}}\alpha[W(t,1)]^p = 0, \quad t > 0, \tag{69}$$

$$\mathcal{L}_4(W,L) = L'(t)\big(1 + W(t,1)\big) + 2\kappa_1\frac{\partial W}{\partial z}(t,1) = 0, \quad t > 0, \tag{70}$$

$$\mathcal{L}_5(Y,L) = L'(t)Y(t,1) + 2\kappa_2\frac{\partial Y}{\partial z}(t,1) = 0, \quad t > 0, \tag{71}$$

and the finite difference scheme (23)–(29), also can be written in a compact way as $\ell(w,y,l) = (\ell_1(w,y,l), \ell_2(w,y,l), \ell_3(w,l), \ell_4(w,l), \ell_5(y,l))$, where:

$$\begin{aligned}\ell_1(w,y,l) \;=\; & l^n\frac{w_j^{n+1} - w_j^n}{k} - \frac{z_j}{2}\frac{w_{j+1}^n - w_{j-1}^n}{2h}\left(\frac{l^{n+1} - l^n}{k}\right) - \kappa_1\frac{w_{j-1}^n - 2w_j^n + w_{j+1}^n}{h^2} \\ & - l^n\beta(\gamma y_j^n - w_j^n) = 0, \quad 0 \le n \le N-1,\ 1 \le j \le M-1,\end{aligned} \tag{72}$$

$$\begin{aligned}\ell_2(w,y,l) \;=\; & l^n\frac{y_j^{n+1} - y_j^n}{k} - \frac{z_j}{2}\frac{y_{j+1}^n - y_{j-1}^n}{2h}\left(\frac{l^{n+1} - l^n}{k}\right) - \kappa_2\frac{y_{j-1}^n - 2y_j^n + y_{j+1}^n}{h^2} \\ & + l^n\beta(\gamma y_j^n - w_j^n) = 0, \quad 0 \le n \le N-1,\ 1 \le j \le M-1,\end{aligned} \tag{73}$$

$$\ell_3(w,l) = \frac{l^{n+1} - l^n}{k} - 2\alpha(l^n)^{\frac{1}{2}}(w_M^n)^p = 0, \quad 0 \le n \le N-1, \tag{74}$$

$$\ell_4(w,l) = \kappa_1\frac{3w_M^n - 4w_{M-1}^n + w_{M-2}^n}{h} + \frac{l^{n+1} - l^n}{k}(1 + w_M^n) = 0, \quad 0 \le n \le N-1, \tag{75}$$

$$\ell_5(y,l) = \kappa_2\frac{3y_M^n - 4y_{M-1}^n + y_{M-2}^n}{h} + \frac{l^{n+1} - l^n}{k}y_M^n = 0, \quad 0 \le n \le N-1. \tag{76}$$

In accordance with [19], scheme $\ell(w,y,l)$ is said to be consistent with problem $\mathcal{L}(W,Y,L)$ if local truncation error $T_j^n(W,Y,L) = (T(1)_j^n, T(2)_j^n, T(3)_j^n, T(4)_j^n, T(5)_j^n)$,

$$T(1)_j^n(W,Y,L) = \ell_1(W_j^n, Y_j^n, L^n) - \mathcal{L}_1(W_j^n, Y_j^n, L^n), \tag{77}$$

$$T(2)_j^n(W,Y,L) = \ell_2(W_n^j, Y_j^n, L^n) - \mathcal{L}_2(W_j^n, Y_j^n, L^n), \tag{78}$$

$$T(3)_j^n(W,L) = \ell_3(W_j^n, L^n) - \mathcal{L}_3(W_j^n, L^n), \tag{79}$$

$$T(4)_j^n(W,L) = \ell_4(W_j^n, L^n) - \mathcal{L}_4(W_j^n, L^n), \tag{80}$$

$$T(5)_j^n(Y,L) = \ell_5(Y_j^n, L^n) - \mathcal{L}_5(Y_j^n, L^n), \tag{81}$$

tends to zero as $k \to 0, h \to 0$, where $W_j^n = W(t^n, z_j)$, $Y_j^n = Y(t^n, z_j)$ and $L^n = L(t^n)$ are the values of the exact solution of problem (11)–(17) of both the PDE and the free boundary respectively at the point (t^n, z_j). We assume that the exact solutions $\{W(t,z), Y(t,z)\}$ are continuously partial differentiable four times with respect to z and two times with respect to t. We also assume that $L(t)$ is two times continuously differentiable.

Let us first consider the components $T(1)_j^n$ and $T(2)_j^n$ of the local truncation error. By using Taylor's expansion about (t^n, z_j) one gets:

$$T(1)_j^n(W,Y,L) = L^nE_j^n(2)k - \frac{z_j}{2}\frac{\partial W}{\partial z}(t^n, z_j)kE^n(1) - \frac{z_j}{2}L'(t^n)E_j^n(3) - \frac{z_j}{2}E^n(1)E_j^n(3)kh^2 - \kappa_1E_j^n(4)h^2, \tag{82}$$

$$T(2)_j^n(W,Y,L) = L^nE_j^n(5)k - \frac{z_j}{2}\frac{\partial Y}{\partial z}(t^n, z_j)kE^n(1) - \frac{z_j}{2}L'(t^n)E_j^n(6) - \frac{z_j}{2}E^n(1)E_j^n(6)kh^2 - \kappa_2E_j^n(7)h^2, \tag{83}$$

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where:

$$E^n(1) = \frac{1}{2}\frac{d^2L}{dt^2}(\tau^1), \qquad E_j^n(2) = \frac{1}{2}\frac{\partial^2 W}{\partial t^2}(\tau^2, z_j), \qquad E_j^n(5) = \frac{1}{2}\frac{\partial^2 Y}{\partial t^2}(\tau^3, z_j),$$
$$t^n < \tau^i < t^{n+1},\ i = 1, 2, 3, \tag{84}$$

$$E_j^n(3) = \frac{1}{6}\frac{\partial^3 W}{\partial z^3}(t^n, \xi_1), \qquad E_j^n(4) = \frac{1}{12}\frac{\partial^4 W}{\partial z^4}(t^n, \xi_2), \qquad E_j^n(6) = \frac{1}{6}\frac{\partial^3 Y}{\partial z^3}(t^n, \xi_3),$$

$$E_j^n(7) = \frac{1}{12}\frac{\partial^4 Y}{\partial z^4}(t^n, \xi_4), \qquad z_{j-1} < \xi_i < z_{j+1}, \quad i = 1, 2, 3, 4, \tag{85}$$

$$E_j^n(8) = \frac{1}{3}\frac{\partial^3 W}{\partial z^3}(t^n, \xi_5), \qquad E_j^n(9) = \frac{1}{3}\frac{\partial^3 Y}{\partial z^3}(t^n, \xi_6), \qquad z_{M-2} < \xi_i < z_M, \quad i = 5, 6. \tag{86}$$

Hence, $T(1)_j^n(W, Y, L)$ and $T(2)_j^n(W, Y, L)$ satisfy

$$T(1)_j^n(W, Y, L) = \mathcal{O}(k) + \mathcal{O}(h^2), \tag{87}$$

$$T(2)_j^n(W, Y, L) = \mathcal{O}(k) + \mathcal{O}(h^2). \tag{88}$$

The remaining components of the truncation error are

$$T(3)_j^n(W, L) = kE^n(1), \tag{89}$$

$$T(4)_j^n(W, L) = kE^n(1)(1 + W(t^n, z_M)) - 2h^2\kappa_1 E_j^n(8), \tag{90}$$

$$T(5)_j^n(Y, L) = kE^n(1)Y(t^n, z_M) - 2h^2\kappa_2 E_j^n(9). \tag{91}$$

Thus, it holds

$$T(3)_j^n(W, L) = \mathcal{O}(k), \tag{92}$$

$$T(4)_j^n(W, L) = \mathcal{O}(k) + \mathcal{O}(h^2), \tag{93}$$

$$T(5)_j^n(Y, L) = \mathcal{O}(k) + \mathcal{O}(h^2). \tag{94}$$

Summarizing, the following result has been established:

Theorem 4. *With previous notation, the scheme $\ell(w, y, l)$ is consistent with the problem $\mathcal{L}(W, Y, L)$ and the local truncation error behaves as:*

$$T_j^n(W, Y, L) = \mathcal{O}(k) + \mathcal{O}(h^2). \tag{95}$$

Remark 1. Note that the coefficients of (35), carbonation front l^{n+1} and the CO_2 concentration in water y_M^n at the propagation front, are distorted by the computation of the CO_2 concentration in air w_M^n at the propagation front, using Newton–Raphson method to solve Eqs. (31)–(32). This means that above we studied the consistency of the scheme resulting of replacing in (23)–(29) the theoretical value w_M^n by the numerical one $\tilde{w}_M^n$ obtained by the Newton–Raphson method. Standard analysis based on the mean value theorem shows that the error of order p motivated by Eq. (30) is linearly transmitted to the other variables adding a local error of order $\mathcal{O}(|w_M^n - \tilde{w}_M^n|^p)$ to the expression (95).

Remark 2. The real initial deterioration state of the concrete in the carbonation process is measured in terms of the value $L(0) = S^2(0) = S_0^2$. This value has influence in the step size conditions (44)–(45) in order to guarantee positivity, stability and monotonicity, that cannot be removed as Example 1 shows. However, this fact does not mean a limitation in our study and its applications, when $S(0)$ is small enough, because starting from any initial position of the carbonation front, using the substitution

$$\tau = \frac{\kappa_1 t}{L(0)}, \qquad \lambda(\tau) = \frac{L(t)}{L(0)}, \tag{96}$$

the problem becomes independent of this situation, as well as of the quality of diffusion given by the coefficient κ_1.

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