# **Uniform Convergent Monotone Iterates for Nonlinear Parabolic Reaction-Diffusion Systems**

#### **Igor Boglaev**

**Abstract** This paper deals with a uniform convergent monotone method for solving nonlinear singularly perturbed parabolic reaction-diffusion systems. The uniform convergence on a piecewise uniform mesh is established. Numerical experiments are presented.

# **1 Introduction**

In this paper we give a numerical treatment for the following semi-linear singularly perturbed parabolic system:

<span id="page-0-0"></span>
$$
\frac{\partial u_i}{\partial t} - \varepsilon_i \frac{\partial^2 u_i}{\partial x^2} + f_i(x, t, u) = 0, \quad (x, t) \in \omega \times (0, T],
$$
  
\n
$$
u_i(0, t) = 0, \quad u_i(1, t) = 0, \quad t \in [0, T],
$$
  
\n
$$
u_i(x, 0) = \psi_i(x), \quad x \in \overline{\omega}, \quad \omega = (0, 1), \quad i = 1, 2,
$$

where  $0 < \varepsilon_1 \leq \varepsilon_2 \leq 1$ ,  $u \equiv (u_1, u_2)$ , the functions  $f_i$  and  $\psi_i$ ,  $i = 1, 2$ , are smooth in their respective domains.

In the study of numerical methods for nonlinear singularly perturbed problems, the two major points to be developed are: (1) constructing robust difference schemes (this means that unlike classical schemes, the error does not increase to infinity, but rather remains bounded, as the small parameters approach zero); (2) obtaining reliable and efficient computing algorithms for solving nonlinear discrete problems. For solving these nonlinear discrete systems, the iterative approach presented in this paper is based on the method of upper and lower solutions and associated monotone iterates. The basic idea of the method of upper and lower solutions is the construction of two monotone sequences which converge monotonically from above

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and below to a solution of the problem. The monotone property of the iterations gives improved upper and lower bounds of the solution in each iteration. An initial iteration in the monotone iterative method is either an upper or lower solution, which can be constructed directly from the difference equation, this method simplifies the search for the initial iteration as is often required in Newton's method.

In [\[5\]](#page-13-0), uniformly convergent numerical methods for solving linear singularly perturbed systems of type [\(1\)](#page-0-0) were constructed. These uniform numerical methods are based on the piecewise uniform meshes of Shishkin-type [\[6\]](#page-13-1).

In [\[2\]](#page-13-2), we investigated uniform convergence properties of the monotone iterative method for solving scalar nonlinear singularly perturbed problems of type [\(1\)](#page-0-0). In this paper, we extend our investigation to the case of the nonlinear singularly perturbed system [\(1\)](#page-0-0).

The structure of the paper as follows. In Sect. [2,](#page-1-0) we introduce a nonlinear difference scheme for solving [\(1\)](#page-0-0). The monotone iterative method is presented in Sect. [3.](#page-2-0) An analysis of the uniform convergence of the monotone iterates to the solution of the nonlinear difference scheme and to the solution of  $(1)$  is given in Sect. [4.](#page-8-0) The final Sect. [5](#page-11-0) presents the results of numerical experiments with a gas-liquid interaction model.

### <span id="page-1-0"></span>**2 The Nonlinear Difference Scheme**

On  $\overline{\omega} = [0, 1]$  and  $[0, T]$ , we introduce meshes  $\overline{\omega}^h$  and  $\overline{\omega}^{\tau}$ :

$$
\overline{\omega}^h = \{x_m, 0 \le m \le M_x; x_0 = 0, x_{M_x} = 1; h_m = x_{m+1} - x_m\},\
$$
  

$$
\overline{\omega}^{\tau} = \{t_k, 0 \le k \le N_{\tau}; t_0 = 0, t_{N_{\tau}} = T; \tau_k = t_k - t_{k-1}\},\
$$

and consider the nonlinear implicit difference scheme

<span id="page-1-1"></span>
$$
\mathcal{L}_i U_i(x_m, t_k) + f_i(x_m, t_k, U) - \tau_k^{-1} U_i(x_m, t_{k-1}) = 0, \quad (x_m, t_k) \in \omega^h \times \omega^\tau,
$$
\n
$$
\mathcal{L}_i U_i(x_m, t_k) \equiv -\varepsilon_i \mathcal{L}_i^h U_i(x_m, t_k) + \tau_k^{-1} U_i(x_m, t_k).
$$
\n
$$
(2)
$$

$$
U_i(x_0, t_k) = U_i(x_{M_x}, t_k) = 0, \quad U_i(x_m, 0) = \psi_i(x_m), \quad x_m \in \overline{\omega}^h, \quad i = 1, 2,
$$

where  $U \equiv (U_1, U_2)$ , and the difference operators  $\mathcal{L}_i^h$ ,  $i = 1, 2$ , are defined by

$$
\mathcal{L}_i^h U_i(x_m, t_k) = \left[ \frac{U_i(x_{m+1}, t_k) - U_i(x_m, t_k)}{\hbar_m h_m} - \frac{U_i(x_m, t_k) - U_i(x_{m-1}, t_k)}{\hbar_m h_{m-1}} \right],
$$
  

$$
\hbar_m = (h_m + h_{m-1})/2, \quad i = 1, 2.
$$

On each time level  $t_k$ ,  $k > 1$ , we introduce the linear problems

<span id="page-2-1"></span>
$$
(\mathcal{L}_i + c_i)W_i(x_m, t_k) = \Phi_i(x_m, t_k), \quad W_i(x_0, t_k) = W_i(x_{M_x}, t_k) = 0,
$$
  

$$
c_i(x_m, t_k) \ge 0, \quad x_m \in \omega^h, \quad i = 1, 2.
$$
 (3)

In the following lemma, we state the maximum principle and we give estimates on solutions of  $(3)$  from  $[8]$ .

#### <span id="page-2-2"></span>**Lemma 1**

*(i)* If mesh functions  $W_i(x_m, t_k)$ ,  $i = 1, 2$ , satisfy the conditions

$$
(\mathcal{L}_i + c_i)W_i(x_m, t_k) \ge 0 \ (\le 0), \quad x_m \in \omega^h,
$$
  

$$
W_i(x_0, t_k) \ge 0 \ (\le 0), \quad W_i(x_{M_x}, t_k) \ge 0 \ (\le 0),
$$

*then*  $W_i(x_m, t_k) \ge 0 \le 0$  *in*  $\overline{\omega}^h$ , *i* = 1, 2*. The following estimates on the solutions* 

*(ii) The following estimates on the solutions of [\(3\)](#page-2-1) hold true*

<span id="page-2-3"></span>
$$
||W_i(\cdot,t_k)||_{\overline{\omega}^h} \leq \max_{x_m \in \omega^h} \left\{ \frac{|\Phi_i(x_m,t_k)|}{c_i(x_m,t_k)+\tau_k^{-1}} \right\}, \quad i=1,2,
$$
 (4)

*where*  $\|W_i(\cdot, t_k)\|_{\overline{\omega}^h} = \max_{x_m \in \overline{\omega}^h} |W_i(x_m, t_k)|$ .

### <span id="page-2-0"></span>**3 The Monotone Iterative Method**

We say that the mesh functions

$$
\widetilde{U}(x_m,t_k)=(\widetilde{U}_1(x_m,t_k),\widetilde{U}_2(x_m,t_k)),\quad \widehat{U}(x_m,t_k)=(\widehat{U}_1(x_m,t_k),\widehat{U}_2(x_m,t_k))
$$

are ordered upper and lower solutions if they satisfy the following inequalities:

$$
\widetilde{U}(x_m, t_k) \geq \widehat{U}(x_m, t_k), \quad (x_m, t_k) \in \overline{\omega}^h \times \omega^\tau,
$$
  

$$
\mathcal{L}_i \widetilde{U}_i(x_m, t_k) + f_i(x_m, t_k, \widetilde{U}) - \tau_k^{-1} \widetilde{U}_i(x_m, t_{k-1}) \geq 0, \quad (x_m, t_k) \in \omega^h \times \omega^\tau,
$$
  

$$
\mathcal{L}_i \widehat{U}_i(x_m, t_k) + f_i(x_m, t_k, \widehat{U}) - \tau_k^{-1} \widehat{U}_i(x_m, t_{k-1}) \leq 0, \quad (x_m, t_k) \in \omega^h \times \omega^\tau,
$$
  

$$
\widehat{U}_i(x_m, t_k) \leq 0 \leq \widetilde{U}_i(x_m, t_k), \quad x_* = x_0, x_{M_x},
$$
  

$$
\widehat{U}_i(x_m, 0) \leq \psi_i(x_m) \leq \widetilde{U}_i(x_m, 0), \quad x_m \in \overline{\omega}^h, \quad i = 1, 2.
$$

We introduce the notation

$$
\langle \widehat{U}(t_k), \widetilde{U}(t_k) \rangle = \{ U(x_m, t_k) : \widehat{U}(x_m, t_k) \leq U(x_m, t_k) \leq \widetilde{U}(x_m, t_k), x_m \in \overline{\omega}^h \},
$$

and we assume that on each time level  $t_k$ ,  $k \geq 1$ , the reaction functions satisfy the assumptions

<span id="page-3-0"></span>
$$
0 \leq \frac{\partial f_i}{\partial u_i}(x_m, t_k, U) \leq c_i(x_m, t_k), \quad \text{on } \langle \widehat{U}(t_k), \widetilde{U}(t_k) \rangle, \tag{5}
$$

$$
0 \leq -\frac{\partial f_i}{\partial u_{i'}}(x_m, t_k, U) \leq q_i(x_m, t_k), \quad \text{on } \langle \widehat{U}(t_k), \widetilde{U}(t_k) \rangle, \quad i' \neq i,
$$

where  $c_i(x_m, t_k)$  and  $q_i(x_m, t_k)$ ,  $i = 1, 2$ , are nonnegative bounded functions in  $\overline{\omega}^h$ .

On each time level  $t_k$ ,  $k \geq 1$ , the iterative method is given in the form

<span id="page-3-1"></span>
$$
(\mathcal{L}_i + c_i)Z_i^{(n)}(x_m, t_k) = -\mathcal{R}_i(x_m, t_k, U^{(n-1)}), \quad x_m \in \omega^h,
$$
 (6)

$$
\mathcal{R}_i(x_m, t_k, U^{(n-1)}) \equiv \mathcal{L}_i U_i^{(n-1)}(x_m, t_k) + f_i(x_m, t_k, U^{(n-1)}) - \tau_k^{-1} U_i(x_m, t_{k-1}),
$$
  

$$
Z_i^{(n)}(x_*, t_k) = 0, \quad n \ge 1, \quad x_* = x_0, x_{M_x},
$$
  

$$
Z_i^{(n)}(x_m, t_k) \equiv U_i^{(n)}(x_m, t_k) - U_i^{(n-1)}(x_m, t_k),
$$
  

$$
U_i(x_m, 0) = \psi_i(x_m), \quad x_m \in \overline{\omega}^h, \quad i = 1, 2,
$$

where  $c_i$ ,  $i = 1, 2$ , are defined in [\(5\)](#page-3-0). For upper sequence, we have  $\overline{U}_i(x_m, 0)$  =  $\psi_i(x_m)$ ,  $\overline{U}^{(0)}(x_m, t_k) = \widetilde{U}_i(x_m, t_k)$  and  $\overline{U}_i(x_m, t_k) = \overline{U}_i^{(n_k)}(x_m, t_k)$ ,  $i = 1, 2, x_m \in \overline{\omega}^h$ ,<br>where  $\overline{U}_i(x_{m+1})$ ,  $i = 1, 2$ , are approximations of the exact solutions on time level where  $\overline{U}_i(x_m, t_k)$ ,  $i = 1, 2$ , are approximations of the exact solutions on time level  $t_k$  and  $n_k$  is a number of iterative steps on time level  $t_k$ . For lower sequence, we have  $\underline{U}_i(x_m, 0) = \psi_i(x_m), \underline{U}^{(0)}(x_m, t_k) = \widehat{U}_i(x_m, t_k)$  and  $\underline{U}(x_m, t_k) = \underline{U}^{(n_k)}(x_m, t_k),$ <br> $i = 1, 2, r \in \overline{\mathbb{Z}}^h$  $i = 1, 2, x_m \in \overline{\omega}^h$ .<br>The following

<span id="page-3-3"></span>The following theorem gives the monotone property of the iterative method [\(6\)](#page-3-1).

**Theorem 1** *Let*  $\widetilde{U}$  and  $\widehat{U}$  be ordered upper and lower solutions, and assumption ([5\)](#page-3-0) *be satisfied. On each time level*  $t_k$ *,*  $k \geq 1$ *, the sequences*  $\{\overline{U}^{(n)}\}$ *,*  $\{\underline{U}^{(n)}\}$  *with*  $\overline{U}^{(0)} = \widetilde{U}$ *<br>and*  $U^{(0)} = \widehat{U}$ *, generated by the iterative method (6), converge monotonically and*  $U^{(0)} = \hat{U}$ , generated by the iterative method ([6\)](#page-3-1), converge monotonically

<span id="page-3-2"></span>
$$
\underline{U}^{(n-1)}(x_m,t_k) \le \underline{U}^{(n)}(x_m,t_k) \le \overline{U}^{(n)}(x_m,t_k) \le \overline{U}^{(n-1)}(x_m,t_k), \quad x_m \in \overline{\omega}^h, \tag{7}
$$

*Proof* Since  $\overline{U}^{(0)} = \widetilde{U}$  and  $\underline{U}^{(0)} = \widehat{U}$ , then from [\(6\)](#page-3-1) we conclude that

$$
(\mathcal{L}_i + c_i) \overline{Z}_i^{(1)}(x_m, t_1) \le 0, \quad (\mathcal{L}_i + c_i) \underline{Z}_i^{(1)}(x_m, t_1) \ge 0, \quad x_m \in \omega^h,
$$
  

$$
\overline{Z}_i^{(1)}(x_*, t_1) \le 0, \quad \underline{Z}_i^{(1)}(x_*, t_1) \ge 0, \quad x_* = x_0, x_{M_x}, \quad i = 1, 2.
$$

From Lemma [1,](#page-2-2) it follows that

<span id="page-4-0"></span>
$$
\overline{Z}_{i}^{(1)}(x_{m}, t_{1}) \leq 0, \quad \underline{Z}_{i}^{(1)}(x_{m}, t_{1}) \geq 0 \quad x_{m} \in \overline{\omega}^{h}, \quad i = 1, 2. \tag{8}
$$

We now prove [\(7\)](#page-3-2) for  $n = 1$  and  $k = 1$ . From [\(6\)](#page-3-1), in the notation  $W_i^{(n)} = \overline{U}_i^{(n)} - \underline{U}_i^{(n)}$ ,  $n > 0$ ,  $i = 1, 2$ , we conclude that  $n > 0$ ,  $i = 1, 2$ , we conclude that

$$
(\mathcal{L}_i + c_i)W_i^{(1)}(x_m, t_1) = F_i(x_m, t_1, \overline{U}^{(0)}) - F_i(x_m, t_1, \underline{U}^{(0)}), \quad x_m \in \omega^h,
$$
  

$$
W_i^{(1)}(x_*, t_1) = 0, \quad x_* = x_0, x_{M_x}, \quad i = 1, 2,
$$

where  $F_i(x_k, t_k, U) = c_i(x_m, t_k)U_i(x_m, t_k) - f_i(x_m, t_k, U)$ . Since  $\overline{U}^{(0)}(x_m, t_1) \geq U^{(0)}(x_m, t_1)$  by Lemma 2 from [1] we conclude that the right hand sides in the  $U^{(0)}(x_m, t_1)$ , by Lemma 2 from [\[1\]](#page-13-4), we conclude that the right hand sides in the difference equations are nonnegative. From Lemma [1,](#page-2-2) it follows  $W_i^{(1)}(p, t_1) \ge 0$ ,  $i - 1, 2$  and this leads to (7) for  $n - 1, k - 1$  $i = 1, 2$ , and this leads to [\(7\)](#page-3-2) for  $n = 1, k = 1$ .

Using the mean-value theorem, from [\(6\)](#page-3-1) we obtain

$$
\mathcal{R}_i(x_m, t_1, \overline{U}^{(1)}) = -\left(c_i - \frac{\partial f_i}{\partial u_i}\right) \overline{Z}_i^{(1)}(x_m, t_1) + \frac{\partial f_i}{\partial u_{i'}} \overline{Z}_{i'}^{(1)}(x_m, t_1), \quad i' \neq i,
$$
(9)

where the partial derivatives are calculated at intermediate points which lie in the sector  $\langle \overline{U}^{(1)}(t_1), \overline{U}^{(0)}(t_1) \rangle$ . From [\(5\)](#page-3-0) and [\(8\)](#page-4-0), we conclude that

$$
\mathcal{R}_i(x_m,t_1,\overline{U}^{(1)}) \geq 0, \quad x_m \in \omega^h, \quad \overline{U}_i^{(1)}(x_*,t_1) = 0, \quad x_* = x_0, x_{M_x}, \ i = 1, 2.
$$

Thus,  $\overline{U}^{(1)}(x_m, t_1)$  is an upper solution. Similarly, we prove that  $U^{(1)}(x_m, t_1)$  is a lower solution. By induction on *n*, we can prove that  $\{\overline{U}^{(n)}(x_m, t_1)\}$  and  $\{\underline{U}^{(n)}(p, t_1)\}$ <br>are respectively monotonically decreasing and monotonically increasing sequences are, respectively monotonically decreasing and monotonically increasing sequences.

From [\(7\)](#page-3-2) with  $t_1$ , it follows that for  $i = 1, 2$ ,

<span id="page-4-1"></span>
$$
\widehat{U}_i(x_m,t_1) \leq \underline{U}_i^{(n_1)}(x_m,t_1) \leq \overline{U}_i^{(n_1)}(x_m,t_1) \leq \widetilde{U}_i(x_m,t_1), \quad x_m \in \overline{\omega}^h. \tag{10}
$$

From here and by the assumption of the theorem that  $U(p, t_2)$  and  $U(p, t_2)$  are, respectively, upper and lower solutions, we conclude that  $U(x_m, t_2)$  and  $U(x_m, t_2)$ are upper and lower solutions with respect to  $\overline{U}^{(n_1)}(x_m, t_1)$  and  $\underline{U}^{(n_1)}(x_m, t_1)$ .

From [\(6\)](#page-3-1), we conclude that  $W^{(1)}(x_m, t_2)$  satisfies

$$
(\mathcal{L}_i + c_i)W_i^{(1)}(x_m, t_2) = F_i(x_m, t_2, \overline{U}^{(0)}) - F_i(x_m, t_2, \underline{U}^{(0)}) + \tau_2^{-1} [\overline{U}_i^{(n_1)}(x_m, t_1) - \underline{U}_i^{(n_1)}(x_m, t_1)],
$$

$$
x_m \in \omega^h
$$
,  $W_i^{(1)}(x_*, t_2) = 0$ ,  $x_* = x_0, x_{M_x}$ ,  $i = 1, 2$ .

Since  $\overline{U}^{(0)}(x_m, t_2) \ge U^{(0)}(x_m, t_2)$  and taking into account [\(10\)](#page-4-1), by Lemma 2 from [\[1\]](#page-13-4), we conclude that the right hand sides in the difference equations are nonnegative. From Lemma [1,](#page-2-2) we have  $W_i^{(1)}(p, t_2) \ge 0$ ,  $i = 1, 2$ , that is,

$$
\underline{U}_i^{(1)}(p,t_2)\leq \overline{U}_i^{(1)}(p,t_2),\quad p\in\overline{\omega}^h,\quad i=1,2.
$$

The proof that  $\overline{U}_i^{(1)}(x_m, t_2)$  and  $\underline{U}_i^{(1)}(x_m, t_2)$ ,  $i = 1, 2$ , are, respectively, upper and lower solutions is similar to the proof on the time level  $t_1$ . By induction on *n*, we can prove that  $\{\overline{U}^{(n)}(x_m, t_2)\}\$  and  $\{\underline{U}^{(n)}(x_m, t_2)\}\$  are, respectively, monotonically<br>decreasing and monotonically increasing sequences decreasing and monotonically increasing sequences.

By induction on *k*,  $k \ge 1$ , we prove that  $\{\overline{U}^{(n)}(x_m, t_k)\}\$  and  $\{\underline{U}^{(n)}(p, t_k)\}\$  are, nectively monotonically decreasing and monotonically increasing sequences respectively, monotonically decreasing and monotonically increasing sequences, which satisfy  $(7)$ .

#### *3.1 Convergence on* [0, T]

We now choose the stopping criterion of the iterative method [\(6\)](#page-3-1) in the form

<span id="page-5-1"></span>
$$
\max_{i} \|\mathcal{R}_{i}(\cdot, t_{k}, U^{(n)})\|_{\omega^{h}} \leq \delta,
$$
\n(11)

where  $\delta$  is a prescribed accuracy, and  $U(x_m, t_k) = U^{(n_k)}(x_m, t_k)$ ,  $x_m \in \overline{\omega}^h$ , where  $n_k$  is minimal subject to the stopping test is minimal subject to the stopping test.

Instead of [\(5\)](#page-3-0), we now impose the two-sided constraints on  $f_i$ ,  $i = 1, 2$ , in the form

<span id="page-5-0"></span>
$$
\rho_k \leq \frac{\partial f_i}{\partial u_i}(x_m, t_k, U) \leq c_i(x_m, t_k), \quad \text{on } \langle \widehat{U}(t_k), \widetilde{U}(t_k) \rangle, \tag{12}
$$

 $0 \leq -\frac{\partial f_i}{\partial u_i}$  $\frac{\partial u_i}{\partial u_{i'}}(x_m, t, U) \leq q_i(x_m, t_k), \text{ on } \langle U(t_k), U(t_k) \rangle, \quad i \neq i',$ 

where  $\rho_k$ ,  $k \geq 1$ , are defined in [\(13\)](#page-6-0).

*Remark 1* We mention that the assumption  $\partial f_i / \partial u_i \ge \rho_k$ ,  $i = 1, 2$ , in [\(12\)](#page-5-0) can always be obtained via a change of variables. Indeed, introduce the following functions  $u_i(x, t) = \exp(\lambda t)z_i(x, t)$ ,  $i = 1, 2$ , where  $\lambda$  is a constant. Now,  $z_i(x, t)$ ,  $i = 1, 2$ , satisfy  $(1)$  with

$$
\varphi_i = \lambda z_i + \exp(-\lambda t) f_i(x, t, \exp(\lambda t) z_1, \exp(\lambda t) z_2),
$$

instead of  $f_i$ ,  $i = 1, 2$ , and we have

$$
\frac{\partial \varphi_i}{\partial z_i} = \lambda + \frac{\partial f_i}{\partial u_i}, \quad \frac{\partial \varphi_i}{\partial z_{i'}} = \frac{\partial f_i}{\partial u_{i'}}, \quad i' \neq i, \quad i = 1, 2.
$$

Thus, if  $\lambda \geq \max_{k>1} \rho_k$ , from here, we conclude that  $\frac{\partial \varphi_i}{\partial z_i}$  and  $\frac{\partial \varphi_i}{\partial z_i}$ satisfy [\(12\)](#page-5-0)

We impose the constraint on  $\tau_k$ 

<span id="page-6-0"></span>
$$
\tau_k < \frac{1}{\rho_k}, \quad \rho_k = \max_i \{ \max_{x_m \in \overline{\omega}^h} [q_i(x_m, t_k)] \}. \tag{13}
$$

If assumptions  $(12)$  and  $(13)$  hold, then the nonlinear difference scheme  $(2)$  has a unique solution (see Lemmas 3 and 4 in [\[1\]](#page-13-4) for details).

<span id="page-6-2"></span>We prove the following convergence result for the iterative method  $(6)$ ,  $(11)$ .

**Theorem 2** Assume that the mesh  $\overline{\omega}^t$  satisfies [\(13\)](#page-6-0), and  $f_i(p, t, U)$ ,  $i = 1, 2,$ *satisfy [\(12\)](#page-5-0), where*  $\widetilde{U}$  *and*  $\widehat{U}$  *are ordered upper and lower solutions of ([2\)](#page-1-1). Then for the sequences*  $\{\overline{U}^{(n)}\}$ ,  $\{\underline{U}^{(n)}\}$ , generated by [\(6\)](#page-3-1), [\(11\)](#page-5-1) with, respectively,  $\overline{U}^{(0)} = \widetilde{U}$ <br>and  $U^{(0)} = \widehat{U}$ , the following uniform in a estimate holds *and*  $U^{(0)} = \hat{U}$ , the following uniform in  $\varepsilon$  estimate holds

<span id="page-6-1"></span>
$$
\max_{i} \left[ \max_{t_k \in \overline{\omega}^t} \| U_i(\cdot, t_k) - U_i^*(\cdot, t_k) \|_{\overline{\omega}^h} \right] \le T\delta,
$$
\n(14)

*where*  $U_i^*(p, t_k)$ ,  $i = 1, 2$ , *is the unique solution to [\(2\)](#page-1-1)*.

*Proof* The difference problem for  $U(x_m, t_k) = U^{(n_k)}(x_m, t_k)$ ,  $k \ge 1$ , can be represented in the form represented in the form

$$
\mathcal{L}_i U_i(x_m, t_k) + f_i(x_m, t_k, U) - \tau_k^{-1} U_i(x_m, t_{k-1}) = \mathcal{R}_i(x_m, t_k, U^{(n_k)}), \quad x_m \in \omega^h,
$$
  

$$
U_i(x_*, t_k) = 0, \quad x_* = x_0, x_{M_x}, \quad i = 1, 2.
$$

From here, [\(2\)](#page-1-1) and using the mean-value theorem, we get the difference problem for  $W_i(x_m, t_k) = U_i(x_m, t_k) - U_i^*(x_m, t_k)$ 

<span id="page-6-3"></span>
$$
\left(\mathcal{L}_i + \frac{\partial f_i}{\partial u_i}\right) W_i(x_m, t_k) = \mathcal{R}_i(x_m, t_k, U) + \frac{1}{\tau_k} W_i(x_m, t_{k-1}) - \frac{\partial f_i}{\partial u_{i'}} W_{i'}(x_m, t_k),
$$
\n
$$
x_m \in \omega^h, \quad W_i(x_*, t_k) = 0, \quad x_* = x_0, x_{M_x} \quad i' \neq i, \quad i = 1, 2,
$$
\n
$$
(15)
$$

where the partial derivatives are calculated at intermediate points  $E_i$ ,  $i = 1, 2$ , such that  $U_i^* \le E_i \le \overline{U}_i^{(0)}$ ,  $i = 1, 2$ , in the case of upper solutions and  $\underline{U}_i^{(0)}$ .<br>*E.*  $\le U_i^*$ ,  $i = 1, 2$ , in the case of lower solutions. Thus, the partial derivation  $E_i \leq U_i^*$ ,  $i = 1, 2$ , in the case of lower solutions. Thus, the partial derivatives<br>  $E_i \leq U_i^*$ ,  $i = 1, 2$ , in the case of lower solutions. Thus, the partial derivatives<br>
satisfy (12) From here (12) using (4) and takin satisfy  $(12)$ . From here,  $(12)$ , using  $(4)$  and taking into account that according to Theorem [1](#page-3-3) the stopping criterion  $(11)$  can always be satisfied, in the notation  $w_k = \max_i \|W_i(\cdot, t_k)\|_{\overline{\omega}^h}$  we have

$$
w_k \leq \frac{1}{\rho_k + \tau_k^{-1}} \left[ \delta + \tau_k^{-1} w_{k-1} + \rho_k w_k \right].
$$

Solving the last inequality for  $w_k$  and taking into account that  $\tau_k^{-1}/(\rho_k + \tau_k^{-1}) > 0$ , we have we have

$$
w_k \leq \delta \tau_k + w_{k-1}.
$$

Since  $w_0 = 0$ , by induction on *k*, we conclude [\(14\)](#page-6-1)

$$
w_k \leq \delta \sum_{l=1}^k \tau_l \leq T\delta, \quad k \geq 1.
$$

# *3.2 Construction of Initial Upper and Lower Solutions*

Here, we give some conditions on functions  $f_i$  and  $\psi_i$ ,  $i = 1, 2$ , to guarantee the existence of upper  $\widetilde{U}$  and lower  $\widehat{U}$  solutions, which are used as the initial iterations in the monotone iterative method  $(6)$ .

*Bounded Reactions Functions* Assume that  $f_i$ ,  $\psi_i$ ,  $i = 1, 2$ , from [\(1\)](#page-0-0) satisfy the conditions

$$
-\sigma_i \le f_i(x,t,0) \le 0, \quad \psi_i(x) \ge 0, \quad u_i(x,t) \ge 0, \quad x \in \overline{\omega},
$$

where  $\sigma_i$ ,  $i = 1, 2$ , are positive constants. Then

$$
\widehat{U}_i(x_m,t_k)=\begin{cases}\psi_i(x_m),\ k=0, & x_m\in\overline{\omega}^h, \quad i=1,2,\\ 0, & k\geq 1,\end{cases}
$$

are lower solutions to [\(2\)](#page-1-1). The solutions of the following linear problems:

$$
\mathcal{L}_i(x_m, t_k) \widetilde{U}_i(x_m, t_k) = \tau_k^{-1} \widetilde{U}_i(x_m, t_{k-1}) + \sigma_i, \quad x_m \in \omega^h, \quad k \ge 1,
$$
  

$$
\widetilde{U}_i(x_*, t_k) = 0, \quad x_* = x_0, x_{M_x}, \quad k \ge 1, \quad \widetilde{U}_i(x_m, 0) = \psi_i(x_m), \quad x_m \in \overline{\omega}^h,
$$

are upper solutions to [\(2\)](#page-1-1).

*Constant Upper and Lower Solutions* Assume that functions  $f_i$ ,  $\psi_i$ ,  $i = 1, 2$ , from [\(1\)](#page-0-0) satisfy the conditions

<span id="page-8-2"></span>
$$
f_i(x, t, 0) \le 0, \quad f_i(x, t, L) \ge 0, \quad \psi_i(x) \ge 0, \quad u_i(x, t) \ge 0, \quad x \in \overline{\omega}, \tag{16}
$$

where  $L = \text{const} > 0$ . The functions

<span id="page-8-3"></span>
$$
\widehat{U}_i(x_m, t_k) = \begin{cases} \psi_i(x_m), \, k = 0, & \widetilde{U}_i(x_m, t_k) = L, & x_m \in \overline{\omega}^h, \\ 0, & k \ge 1, \end{cases}
$$
\n(17)

are, respectively, lower and upper solutions.

#### <span id="page-8-0"></span>**4 Uniform Convergence of the Monotone Iterates**

We assume that  $0 < \varepsilon_1 < \varepsilon_2 < 1$ .

In the notation  $u = (u_1, u_2), \varepsilon = (\varepsilon_1, \varepsilon_2)$  and  $f = (f_1, f_2)$ , the following linear system is considered in [\[5\]](#page-13-0):

$$
\frac{\partial u}{\partial t} - \varepsilon \frac{\partial^2 u}{\partial x^2} + A(x, t)u = f(x, t), \quad A(x, t) = \begin{bmatrix} a_{11}(x, t) & a_{12}(x, t) \\ a_{21}(x, t) & a_{22}(x, t) \end{bmatrix},
$$

where the matrix  $A(x, t)$  satisfies the assumptions

$$
a_{ii}(x,t) > 0, \qquad a_{ii'}(x,t) \le 0, \quad a_{ii}(x,t) + a_{ii'}(x,t) \ge \alpha = \text{const} > 0,
$$
\n
$$
i \ne i', \quad i = 1, 2, \quad (x,t) \in \overline{\omega} \times [0,T].
$$

From [\[5\]](#page-13-0), we write down the bounds on  $\partial u_i/\partial x$ ,  $i = 1, 2$  in the form

<span id="page-8-1"></span>
$$
\left|\frac{\partial u_1}{\partial x}(x,t)\right| \le C\left[1 + \mu_1^{-1}\pi_{\mu_1}(x) + \mu_2^{-1}\pi_{\mu_2}(x)\right],\tag{18}
$$

$$
\left|\frac{\partial u_2}{\partial x}(x,t)\right| \le C\left[1 + \mu_2^{-1}\pi_{\mu_2}(x)\right], \quad \pi_\gamma(x) \equiv \exp(-\gamma^{-1}x) + \exp(-\gamma^{-1}(1-x)),
$$

where  $\mu_i = \sqrt{\varepsilon_i}$ ,  $i = 1, 2$ , and  $\gamma$  is a positive constant. These bounds show that there are two overlapping boundary layers at  $x = 0$  and  $x = 1$ .

By using the mean-value theorem, we write  $f_i$ ,  $i = 1, 2$ , from [\(1\)](#page-0-0) in the form

$$
f_i(x,t,u) = f_i(x,t,0) + \frac{\partial f_i}{\partial u_i}(x,t,v)u_i + \frac{\partial f_i}{\partial u_{i'}}(x,t,v)u_{i'}, \quad i' \neq i, \quad i, i' = 1,2,
$$

where *v* lies between 0 and *u*. We suppose that  $\partial f_i / \partial u_i$  and  $\partial f_i / \partial u_{i'}, i' \neq i, i, i'$ <br>1 2 for  $(x, t, v) \in \overline{\omega} \times [0, T] \times (-\infty, \infty)$  satisfy the following assumptions: 1, 2, for  $(x, t, v) \in \overline{\omega} \times [0, T] \times (-\infty, \infty)$  satisfy the following assumptions:

<span id="page-9-0"></span>
$$
\frac{\partial f_i}{\partial u_i}(x, t, v) > 0, \quad \frac{\partial f_i}{\partial u_{i'}}(x, t, v) \le 0, \quad i' \ne i, \quad i, i' = 1, 2,\tag{19}
$$

$$
\min_{-\infty \le v \le \infty} \left[ \frac{\partial f_i}{\partial u_i}(x, t, v) + \frac{\partial f_i}{\partial u_{i'}}(x, t, v) \right] > \alpha = \text{const} > 0.
$$

*Remark 2* If assumptions [\(19\)](#page-9-0) hold, then Theorem 3.1, Chap. 8 in [\[7\]](#page-13-5) guarantees existence and uniqueness of the solution to problem  $(1)$ .

We may now consider  $(1)$  as a linear problem and use bounds  $(18)$  on the exact solutions. We introduce the piecewise uniform mesh  $\overline{\omega}^h$  of Shishkin-type from [\[5\]](#page-13-0), where the boundary layer thicknesses  $\zeta_{\varepsilon_i}$ ,  $i = 1, 2$ , and mesh spacings  $h_{\varepsilon_i}$ ,  $i = 1, 2$ ,  $h$  are defined by *h* are defined by

<span id="page-9-1"></span>
$$
\zeta_{\varepsilon_2} = \min\left\{1/4, 2\sqrt{\varepsilon_2}\ln M_x\right\}, \quad \zeta_{\varepsilon_1} = \min\left\{\zeta_{\varepsilon_2}/2, 2\sqrt{\varepsilon_1}\ln M_x\right\},\tag{20}
$$
\n
$$
h_{\varepsilon_1} = 8\zeta_{\varepsilon_1}/M_x, \quad h_{\varepsilon_2} = 8(\zeta_{\varepsilon_2} - \zeta_{\varepsilon_1})/M_x \quad h = 2(1 - 2\zeta_{\varepsilon_2})/M_x.
$$

The mesh  $\overline{\omega}^h$  is constructed thus: in each of the subintervals  $[0, \zeta_{\varepsilon_1}]$ ,  $[\zeta_{\varepsilon_1}, \zeta_{\varepsilon_2}]$ ,  $[\zeta_{\varepsilon_2}, 1 - \zeta_{\varepsilon_2}]$ ,  $[1 - \zeta_{\varepsilon_2}, 1 - \zeta_{\varepsilon_1}]$  and  $[1 - \zeta_{\varepsilon_1}, 1]$ , mesh points are distributed uniformly<br>with M (8+1 M (8+1 M (2+1 M (8+1 and M (8+1 mesh points respectively with  $M_x/8+1$ ,  $M_x/8+1$ ,  $M_x/2+1$ ,  $M_x/8+1$  and  $M_x/8+1$  mesh points, respectively. The mesh spacings  $h_{\varepsilon_1}$ ,  $h_{\varepsilon_2}$  and *h* are in use, respectively, in the first and last, in the second and fourth, in the third domains.

<span id="page-9-2"></span>**Theorem 3** Assume that meshes  $\overline{\omega}^t$  and  $\overline{\omega}^h$  satisfy, respectively, [\(13\)](#page-6-0) and [\(20\)](#page-9-1), and  $f_i(x, t, u)$ ,  $i = 1, 2$ , satisfy [\(19\)](#page-9-0). Then the nonlinear difference scheme [\(2\)](#page-1-1) converges  $\varepsilon$ -uniformly to the solution of  $(1)$ 

$$
\max_{i} \left[ \max_{t_k \in \overline{\omega}^{\tau}} \| U_i^*(\cdot, t_k) - u_i^*(\cdot, t_k) \|_{\overline{\omega}^h} \right] \leq C(M_x^{-1} \ln M_x + \tau), \quad \tau = \max_k \tau_k, \quad (21)
$$

*where*  $U_i^*$  *and*  $u_i^*$ *, i* = 1, 2*, are, respectively, the exact solutions to [\(2\)](#page-1-1) and [\(1\)](#page-0-0), C is a generic constant which is independent of s. M. and*  $\tau$ *a generic constant which is independent of*  $\varepsilon$ *,*  $M_x$  *and*  $\tau$ *.* 

*Proof* Since the proof of the theorem follows the proof of Theorem 1 from [\[3\]](#page-13-6), then we only present the sketch of it.

The exact solutions  $u_i^*(x, t)$ ,  $i = 1, 2$ , can be presented on  $[x_{m-1}, x_{m+1}]$  in the paral-difference form (compare with (5) from [3]) integral-difference form (compare with (5) from [\[3\]](#page-13-6))

$$
\varepsilon_i \mathcal{L}_i^h u_i^*(x_m, t_k) = \frac{\partial u_i^*}{\partial t} + f_i(x_m, t_k, u^*) + I_i(x_m, t_k, u^*), \quad x_m, t_k \in \omega^h \times \omega^\tau,
$$

where  $u^* = (u_1^*, u_2^*), \mathcal{L}_i^h, i = 1, 2$ , are defined in [\(2\)](#page-1-1) and  $I_i, i = 1, 2$ , are given in the form the form

$$
I_i(x_m, t_k, u^*) = \frac{1}{\hbar_m} \int_{x_{m-1}}^{x_m} \phi_{2,m-1}(s) \left( \int_{x_m}^s \frac{d\psi_i(\xi, t_k)}{d\xi} d\xi \right) ds + \frac{1}{\hbar_m} \int_{x_m}^{x_{m+1}} \phi_{1,m}(s) \left( \int_{x_m}^s \frac{d\psi_i(\xi, t_k)}{d\xi} d\xi \right) ds, \n\psi_i(x, t_k) = f_i(x, t_k, u^*) + \frac{\partial u_i^*(x, t_k)}{\partial t}, \quad x \in [x_{m-1}, x_{m+1}], \n\phi_{1,m}(x) = \frac{x_{m+1} - x}{\hbar_m}, \quad \phi_{2,m}(x) = \frac{x - x_m}{\hbar_m},
$$

The truncation errors  $T_i(x_m, t_k)$ ,  $i = 1, 2$ , can be represented in the form

$$
T_i(x_m, t_k) = T_{i,1}(x_m, t_k) - I_i(x_m, t_k, u^*),
$$
  

$$
T_{i,1}(x_m, t_k) = \frac{u_i^*(x_m, t_k) - u_i^*(x_m, t_{k-1})}{\tau_k} - \frac{\partial u_i^*(x_m, t_k)}{\partial t}.
$$

Using the Taylor expansion about  $(x_m, t_k)$ , we obtain

<span id="page-10-0"></span>
$$
||T_i(\cdot,t_k)||_{\omega^h} \leq \frac{1}{2} \max_{(x,t)\in Q} |u_{i,t}^*|\tau_k + ||I_i(\cdot,t_k)||_{\omega^h}.
$$
 (22)

Thus, similar to [\[3\]](#page-13-6), using bounds [\(18\)](#page-8-1), the following estimates on  $d\psi_i/dx$ ,  $i=1,2$ , hold true

$$
\left|\frac{d\psi_i(x,t)}{dx}\right| \le C\left[1+\mu_1^{-1}\pi_{\mu_1}(x)+\mu_2^{-1}\pi_{\mu_2}(x)\right], \quad i=1,2.
$$

From here, using the properties of the piecewise uniform mesh of Shishkin-type and repeating the proof of Theorem 1 from [\[3\]](#page-13-6), we prove the estimates

$$
||I_i(\cdot,t_k)||_{\omega^h}\leq C\left(M_{x}^{-1}\ln M_{x}\right),\quad i=1,2.
$$

From here and  $(22)$ , we obtain

$$
||T_i(\cdot,t_k)||_{\omega^h}\leq C\left(M_x^{-1}\ln M_x+\tau\right),\quad i=1,2.
$$

The difference problems for  $u_i^*$ ,  $i = 1, 2$ , can be represented in the form

$$
\mathcal{L}_i u_i^*(x_m, t_k) + f_i(x_m, t_k, u^*) - \tau_k^{-1} u_i^*(x_m, t_{k-1}) = T_i(x_m, t_k), \quad x_m \in \omega^h,
$$
  

$$
u_i^*(x_*, t_k) = 0, \quad x_* = x_0, x_{M_x}, \quad i = 1, 2.
$$

From here, [\(2\)](#page-1-1) and using the mean-value theorem, we get the difference problem for  $W_i(x_m, t_k) = U_i(x_m, t_k) - u_i^*(x_m, t_k)$  in the form

$$
\left(\mathcal{L}_i + \frac{\partial f_i}{\partial u_i}\right) W_i(x_m, t_k) = -T_i(x_m, t_k) + \frac{1}{\tau_k} W_i(x_m, t_{k-1}) - \frac{\partial f_i}{\partial u_{i'}} W_{i'}(x_m, t_k),
$$
  

$$
x_m \in \omega^h, \quad W_i(x_*, t_k) = 0, \quad x_* = x_0, x_{M_x} \quad i' \neq i, \quad i = 1, 2.
$$

Now the proof of the theorem repeats the proof of Theorem [2](#page-6-2) starting from [\(15\)](#page-6-3), where  $-T_i$ ,  $i = 1, 2$ , are in use instead of  $\mathcal{R}_i$ ,  $i = 1, 2$ , in [\(15\)](#page-6-3).

**Theorem 4** *Assume that all the assumptions in Theorem [3](#page-9-2) are satisfied. Then for the sequences*  $\{\overline{U}^{(n)}\}$  *and*  $\{\underline{U}^{(n)}\}$ *, generated by [\(6\)](#page-3-1), [\(11\)](#page-5-1) with, respectively,*  $\overline{U}^{(0)} = \widetilde{U}$ <br>and  $U^{(0)} = \widehat{U}$ , the uniform in a estimate holds *and*  $U^{(0)} = \widehat{U}$ , the uniform in  $\varepsilon$  estimate holds

$$
\max_{i}\left[\max_{t_k\in\overline{\omega}^{\tau}}\|U_i(\cdot,t_k)-u_i^*(\cdot,t_k)\|_{\overline{\omega}^h}\right]\leq C(\delta+M_{x}^{-1}\ln M_{x}+\tau),
$$

*where*  $U_i(p, t_k) = \overline{U}^{(n_k)}(p, t_k)$  or  $U_i(p, t_k) = \underline{U}^{(n_k)}(p, t_k)$  and  $u_i^*, i = 1, 2$ , are the exact solutions to (1) *exact solutions to [\(1\)](#page-0-0).*

*Proof* The proof of the theorem follows from Theorems [2](#page-6-2) and [3.](#page-9-2)

# <span id="page-11-0"></span>**5 Gas-Liquid Interaction Model**

The gas-liquid interaction model in the non-dimensional variables can be presented in the form (see [\[4\]](#page-13-7) for details)

$$
\frac{\partial u_1}{\partial t} - \frac{\partial u_1}{\partial x^2} - \kappa_1 (1 - u_1) u_2 = 0, \quad (x, t) \in \omega \times (0, T],
$$
  

$$
\frac{\partial u_2}{\partial t} - \varepsilon \frac{\partial u_2}{\partial x^2} + \kappa_2 (1 - u_1) u_2 = 0, \quad (x, t) \in \omega \times (0, T],
$$
  

$$
u_1(0, t) = u_1(1, t) = 0, \quad u_2(0, t) = u_2(1, t) = 1,
$$
  

$$
u_1(x, 0) = 0, \quad u_2(x, 0) = \sin(\pi x), \quad x \in \overline{\omega},
$$

where  $u_1$  and  $u_2$  are, respectively, concentrations of a dissolved gas and a dissolved reactant and  $\kappa_i$ ,  $i = 1, 2$ , are positive constants. The test problem, which corresponds to the case  $\varepsilon_1 = 1$ ,  $\varepsilon_2 = \varepsilon$ , for small values of  $\varepsilon$  is singularly perturbed and  $u_2$  has boundary layers of width  $\mathcal{O}(\sqrt{\varepsilon})$  near  $x = 0$  and  $x = 1$ .

It is easy to verify that assumptions [\(16\)](#page-8-2) with  $L<sub>i</sub> = 1, i = 1, 2$ , hold true. Thus, *U<sub>i</sub>* and *U<sub>i</sub>*,  $i = 1, 2$ , from [\(17\)](#page-8-3) are, respectively, lower and upper solutions to the test problem. From here it follows that the inequalities in (12) hold, and one can choose problem. From here, it follows that the inequalities in [\(12\)](#page-5-0) hold, and one can choose  $c_i(x_m, t_k) = \kappa_i$ ,  $i = 1, 2$ , in (5) The exact solution is not available, so we estimate  $c_i(x_m, t_k) = \kappa_i$ ,  $i = 1, 2$ , in [\(5\)](#page-3-0) The exact solution is not available, so we estimate<br>the error of the numerical solutions  $U_i^{M_x}$ ,  $i = 1, 2$ , with respect to the reference<br>solutions  $U_i^{2M_x}$ ,  $i = 1, 2$ solutions  $U_i^{2M_x}$ ,  $i = 1, 2$ ,

$$
E_{M_x} = \max_{i=1,2} \| U_i^{M_x}(\cdot,t_{N_\tau}) - U_i^{2M_x}(\cdot,t_{N_\tau}) \|_{\overline{\omega}^h},
$$

and assume that  $E_{M_x} = C(1/M_x)^{p_{M_x}}$ , where constant *C* is independent of  $M_x$ , and  $p_{M_x}$  is the order of maximum numerical error. For each  $M_x$ , we compute  $p_{M_x}$  from

$$
p_{M_x}=\log_2\frac{E_{M_x}}{E_{2M_x}}.
$$

We choose  $\delta = 10^{-8}$  in the stopping test [\(11\)](#page-5-1). In Table [1,](#page-12-0) for parameters  $\kappa_i = 1$ ,  $i = 1, 2, t_v = 0.5$ ,  $\tau = 5 \times 10^{-4}$  and different values of  $\varepsilon$  and M, we present the  $i = 1, 2, t_{N<sub>t</sub>} = 0.5, \tau = 5 \times 10^{-4}$  and different values of  $\varepsilon$  and  $M_x$ , we present the maximum numerical error  $B_x$  and the maximum numerical error  $E_{M_x}$ , the order of maximum numerical error  $p_{M_x}$  and the number of monotone iterations  $n_{M_x}$  on each time level. The data in the table show that for  $\varepsilon \leq 10^{-4}$ , the numerical solution converges uniformly in  $\varepsilon$ , has the first-<br>order accuracy in the space variable, and the monotone sequences converge in few order accuracy in the space variable, and the monotone sequences converge in few iterations.

<span id="page-12-0"></span>

	32	64	128	256	512
$E_{M_r}$	$5.949e - 5$	$2.046e - 5$	$8.296e - 6$	$3.712e - 6$	$1.753e - 6$
$p_{M_x}$	1.539	1.302	1.160	1.081	
$n_{M_{r}}$	2	2	$\mathbf{1}$	$\mathbf{1}$	$\mathbf{1}$
$E_{M_x}$	$4.265e - 4$	$1.684e - 4$	$7.054e - 5$	$3.280e - 5$	$1.583e - 5$
$p_{M_x}$	1.341	1.255	1.105	1.051	
$n_{M_{Y}}$	2	2	$\mathbf{1}$	$\mathbf{1}$	$\mathbf{1}$
$E_{M_{\underline{x}}}$	$2.001e - 3$	$9.127e - 4$	$4.293e - 4$	$2.078e - 4$	$1.021e - 4$
$p_{M_x}$	1.133	1.088	1.047	1.025	
$n_{M_x}$	3	3	$\overline{2}$	2	2
$E_{M_r}$	$2.058e - 3$	$9.371e - 4$	$4.411e - 4$	$2.135e - 4$	$1.049e - 4$
$p_{M_x}$	1.135	1.087	1.047	1.025	
$n_{M_x}$	3	3	$\overline{2}$	2	2
$E_{M_r}$	$2.103e - 3$	$9.557e - 4$	$4.498e - 4$	$2.177e - 4$	$1.070e - 4$
$p_{M_x}$	1.138	1.087	1.047	1.024	
$n_{M_x}$	3	3	2	2	2

**Table 1** Numerical results

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