Uniform Convergent Monotone Iterates for Nonlinear Parabolic Reaction-Diffusion Systems

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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:

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

where $0 < \varepsilon_1 \le \varepsilon_2 \le 1$, $u \equiv (u_1, u_2)$, the functions f_i and ψ_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], uniformly convergent numerical methods for solving linear singularly perturbed systems of type (1) were constructed. These uniform numerical methods are based on the piecewise uniform meshes of Shishkin-type [6].

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

The structure of the paper as follows. In Sect. 2, we introduce a nonlinear difference scheme for solving (1). The monotone iterative method is presented in Sect. 3. 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. The final Sect. 5 presents the results of numerical experiments with a gas-liquid interaction model.

2 The Nonlinear Difference Scheme

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

$$\overline{\omega}^{h} = \{x_{m}, 0 \le m \le M_{x}; x_{0} = 0, x_{M_{x}} = 1; h_{m} = x_{m+1} - x_{m}\},\$$
$$\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

$$\mathcal{L}_{i}U_{i}(x_{m},t_{k}) + f_{i}(x_{m},t_{k},U) - \tau_{k}^{-1}U_{i}(x_{m},t_{k-1}) = 0, \quad (x_{m},t_{k}) \in \omega^{h} \times \omega^{\tau},$$
(2)
$$\mathcal{L}_{i}U_{i}(x_{m},t_{k}) \equiv -\varepsilon_{i}\mathcal{L}_{i}^{h}U_{i}(x_{m},t_{k}) + \tau_{k}^{-1}U_{i}(x_{m},t_{k}).$$

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

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 , $k \ge 1$, we introduce the linear problems

$$(\mathcal{L}_{i} + c_{i})W_{i}(x_{m}, t_{k}) = \Phi_{i}(x_{m}, t_{k}), \quad W_{i}(x_{0}, t_{k}) = W_{i}(x_{M_{x}}, t_{k}) = 0,$$
(3)
$$c_{i}(x_{m}, t_{k}) \geq 0, \quad x_{m} \in \omega^{h}, \quad i = 1, 2.$$

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

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.

(ii) The following estimates on the solutions of (3) hold true

$$\|W_{i}(\cdot, t_{k})\|_{\overline{\omega}^{h}} \leq \max_{x_{m} \in \omega^{h}} \left\{ \frac{|\Phi_{i}(x_{m}, t_{k})|}{c_{i}(x_{m}, t_{k}) + \tau_{k}^{-1}} \right\}, \quad i = 1, 2,$$
(4)

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

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:

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

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

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

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

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

We introduce the notation

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

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

$$0 \leq \frac{\partial f_i}{\partial u_i}(x_m, t_k, U) \leq c_i(x_m, t_k), \quad \text{on } \langle \widehat{U}(t_k), \widetilde{U}(t_k) \rangle, \tag{5}$$
$$0 \leq -\frac{\partial f_i}{\partial u_{i'}}(x_m, t_k, U) \leq q_i(x_m, t_k), \quad \text{on } \langle \widehat{U}(t_k), \widetilde{U}(t_k) \rangle, \quad i' \neq i,$$

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 , $k \ge 1$, the iterative method is given in the form

$$(\mathcal{L}_i + c_i) Z_i^{(n)}(x_m, t_k) = -\mathcal{R}_i(x_m, t_k, U^{(n-1)}), \quad x_m \in \omega^h,$$
(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). 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 $\overline{U}_i(x_m, t_k) = \overline{U}_i^{(n_k)}(x_m, t_k)$, $i = 1, 2, x_m \in \overline{\omega}^h$, 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 $\underline{U}(x_m, t_k) = \underline{U}^{(n_k)}(x_m, t_k)$, $i = 1, 2, x_m \in \overline{\omega}^h$.

The following theorem gives the monotone property of the iterative method (6).

Theorem 1 Let \widetilde{U} and \widehat{U} be ordered upper and lower solutions, and assumption (5) be satisfied. On each time level t_k , $k \ge 1$, the sequences $\{\overline{U}^{(n)}\}, \{\underline{U}^{(n)}\}$ with $\overline{U}^{(0)} = \widetilde{U}$ and $\underline{U}^{(0)} = \widehat{U}$, generated by the iterative method (6), converge monotonically

$$\underline{U}^{(n-1)}(x_m, t_k) \leq \underline{U}^{(n)}(x_m, t_k) \leq \overline{U}^{(n)}(x_m, t_k) \leq \overline{U}^{(n-1)}(x_m, t_k), \quad x_m \in \overline{\omega}^h,$$
(7)

Proof Since $\overline{U}^{(0)} = \widetilde{U}$ and $\underline{U}^{(0)} = \widehat{U}$, then from (6) we conclude that

$$(\mathcal{L}_{i}+c_{i})\overline{Z}_{i}^{(1)}(x_{m},t_{1}) \leq 0, \quad (\mathcal{L}_{i}+c_{i})\underline{Z}_{i}^{(1)}(x_{m},t_{1}) \geq 0, \quad x_{m} \in \omega^{h},$$

$$\overline{Z}_{i}^{(1)}(x_{*},t_{1}) \leq 0, \quad \underline{Z}_{i}^{(1)}(x_{*},t_{1}) \geq 0, \quad x_{*}=x_{0}, x_{M_{x}}, \quad i=1,2.$$

From Lemma 1, it follows that

$$\overline{Z}_{i}^{(1)}(x_{m},t_{1}) \leq 0, \quad \underline{Z}_{i}^{(1)}(x_{m},t_{1}) \geq 0 \quad x_{m} \in \overline{\omega}^{h}, \quad i = 1, 2.$$
(8)

We now prove (7) for n = 1 and k = 1. From (6), in the notation $W_i^{(n)} = \overline{U}_i^{(n)} - \underline{U}_i^{(n)}$, $n \ge 0, i = 1, 2$, 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 $\overline{U}^{(0)}(x_m, t_1) \ge \underline{U}^{(0)}(x_m, t_1)$, by Lemma 2 from [1], we conclude that the right hand sides in the difference equations are nonnegative. From Lemma 1, it follows $W_i^{(1)}(p, t_1) \ge 0$, i = 1, 2, and this leads to (7) for n = 1, k = 1.

Using the mean-value theorem, from (6) 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) and (8), we conclude that

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

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

From (7) with t_1 , it follows that for i = 1, 2,

$$\widehat{U}_i(x_m, t_1) \le \underline{U}_i^{(n_1)}(x_m, t_1) \le \overline{U}_i^{(n_1)}(x_m, t_1) \le \widetilde{U}_i(x_m, t_1), \quad x_m \in \overline{\omega}^h.$$
(10)

From here and by the assumption of the theorem that $\widetilde{U}(p, t_2)$ and $\widehat{U}(p, t_2)$ are, respectively, upper and lower solutions, we conclude that $\widetilde{U}(x_m, t_2)$ and $\widehat{U}(x_m, t_2)$ 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), 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 $\overline{U}^{(0)}(x_m, t_2) \ge \underline{U}^{(0)}(x_m, t_2)$ and taking into account (10), by Lemma 2 from [1], we conclude that the right hand sides in the difference equations are nonnegative. From Lemma 1, 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 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, 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) in the form

$$\max_{i} \|\mathcal{R}_{i}(\cdot, t_{k}, U^{(n)})\|_{\omega^{h}} \leq \delta,$$
(11)

where δ 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.

Instead of (5), we now impose the two-sided constraints on f_i , i = 1, 2, in the form

$$\rho_{k} \leq \frac{\partial f_{i}}{\partial u_{i}}(x_{m}, t_{k}, U) \leq c_{i}(x_{m}, t_{k}), \quad \text{on } \langle \widehat{U}(t_{k}), \widetilde{U}(t_{k}) \rangle, \tag{12}$$
$$\leq -\frac{\partial f_{i}}{\partial u_{i}}(x_{m}, t, U) \leq q_{i}(x_{m}, t_{k}), \quad \text{on } \langle \widehat{U}(t_{k}), \widetilde{U}(t_{k}) \rangle, \quad i \neq i',$$

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

where $\rho_k, k \ge 1$, are defined in (13).

Remark 1 We mention that the assumption $\partial f_i / \partial u_i \ge \rho_k$, i = 1, 2, in (12) 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 λ 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 $\lambda \geq \max_{k\geq 1} \rho_k$, from here, we conclude that $\partial \varphi_i / \partial z_i$ and $\partial \varphi_i / \partial z_{i'}$ satisfy (12)

We impose the constraint on τ_k

$$\tau_k < \frac{1}{\rho_k}, \quad \rho_k = \max_i \{ \max_{x_m \in \overline{\omega}^h} [q_i(x_m, t_k)] \}.$$
(13)

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

We prove the following convergence result for the iterative method (6), (11).

Theorem 2 Assume that the mesh $\overline{\omega}^{\tau}$ satisfies (13), and $f_i(p, t, U)$, i = 1, 2, satisfy (12), where \widetilde{U} and \widehat{U} are ordered upper and lower solutions of (2). Then for the sequences $\{\overline{U}^{(n)}\}, \{\underline{U}^{(n)}\}$, generated by (6), (11) with, respectively, $\overline{U}^{(0)} = \widetilde{U}$ and $\underline{U}^{(0)} = \widehat{U}$, the following uniform in ε estimate holds

$$\max_{i} \left[\max_{t_k \in \overline{\omega}^i} \| U_i(\cdot, t_k) - U_i^*(\cdot, t_k) \|_{\overline{\omega}^h} \right] \le T\delta,$$
(14)

where $U_i^*(p, t_k)$, i = 1, 2, is the unique solution to (2).

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

$$\mathcal{L}_{i}U_{i}(x_{m}, t_{k}) + f_{i}(x_{m}, t_{k}, U) - \tau_{k}^{-1}U_{i}(x_{m}, t_{k-1}) = \mathcal{R}_{i}(x_{m}, t_{k}, U^{(n_{k})}), \quad x_{m} \in \omega^{h},$$
$$U_{i}(x_{*}, t_{k}) = 0, \quad x_{*} = x_{0}, x_{M_{*}}, \quad i = 1, 2.$$

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

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

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

$$(15)$$

where the partial derivatives are calculated at intermediate points E_i , i = 1, 2, such that $U_i^* \leq E_i \leq \overline{U}_i^{(0)}$, i = 1, 2, in the case of upper solutions and $\underline{U}_i^{(0)} \leq E_i \leq U_i^*$, i = 1, 2, in the case of lower solutions. Thus, the partial derivatives satisfy (12). From here, (12), using (4) and taking into account that according to Theorem 1 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

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

Since $w_0 = 0$, by induction on k, we conclude (14)

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

3.2 Construction of Initial Upper and Lower Solutions

Here, we give some conditions on functions f_i and ψ_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 , ψ_i , i = 1, 2, from (1) satisfy the conditions

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

where σ_i , i = 1, 2, are positive constants. Then

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

are lower solutions to (2). 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).

Constant Upper and Lower Solutions Assume that functions f_i , ψ_i , i = 1, 2, from (1) satisfy the conditions

$$f_i(x,t,0) \le 0, \quad f_i(x,t,L) \ge 0, \quad \psi_i(x) \ge 0, \quad u_i(x,t) \ge 0, \quad x \in \overline{\omega}, \tag{16}$$

where L = const > 0. The functions

$$\widehat{U}_i(x_m, t_k) = \begin{cases} \psi_i(x_m), \, k = 0, \\ 0, \quad k \ge 1, \end{cases} \qquad \widetilde{U}_i(x_m, t_k) = L, \quad x_m \in \overline{\omega}^h, \tag{17}$$

are, respectively, lower and upper solutions.

4 Uniform Convergence of the Monotone Iterates

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

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]:

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

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

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

From [5], we write down the bounds on $\partial u_i / \partial x$, i = 1, 2 in the form

$$\left|\frac{\partial u_1}{\partial x}(x,t)\right| \le C \left[1 + \mu_1^{-1} \pi_{\mu_1}(x) + \mu_2^{-1} \pi_{\mu_2}(x)\right],\tag{18}$$

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

where $\mu_i = \sqrt{\varepsilon_i}$, i = 1, 2, and γ 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) 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' = 1, 2, for $(x, t, v) \in \overline{\omega} \times [0, T] \times (-\infty, \infty)$ satisfy the following assumptions:

$$\frac{\partial f_i}{\partial u_i}(x,t,v) > 0, \quad \frac{\partial f_i}{\partial u_{i'}}(x,t,v) \le 0, \qquad i' \ne i, \quad i,i' = 1,2, \tag{19}$$

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

Remark 2 If assumptions (19) hold, then Theorem 3.1, Chap. 8 in [7] 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], where the boundary layer thicknesses ζ_{ε_i} , i = 1, 2, and mesh spacings h_{ε_i} , i = 1, 2, h are defined by

$$\varsigma_{\varepsilon_2} = \min\left\{1/4, 2\sqrt{\varepsilon_2}\ln M_x\right\}, \quad \varsigma_{\varepsilon_1} = \min\left\{\varsigma_{\varepsilon_2}/2, 2\sqrt{\varepsilon_1}\ln M_x\right\}, \tag{20}$$

$$h_{\varepsilon_1} = 8_{\varsigma_{\varepsilon_1}}/M_x, \quad h_{\varepsilon_2} = 8(\varsigma_{\varepsilon_2} - \varsigma_{\varepsilon_1})/M_x \quad h = 2(1 - 2\varsigma_{\varepsilon_2})/M_x.$$

The mesh $\overline{\omega}^h$ is constructed thus: in each of the subintervals $[0, \varsigma_{\varepsilon_1}]$, $[\varsigma_{\varepsilon_1}, \varsigma_{\varepsilon_2}]$, $[\varsigma_{\varepsilon_2}, 1-\varsigma_{\varepsilon_2}]$, $[1-\varsigma_{\varepsilon_2}, 1-\varsigma_{\varepsilon_1}]$ and $[1-\varsigma_{\varepsilon_1}, 1]$, mesh points are distributed uniformly 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_{ε_1} , h_{ε_2} and h are in use, respectively, in the first and last, in the second and fourth, in the third domains.

Theorem 3 Assume that meshes $\overline{\omega}^{\tau}$ and $\overline{\omega}^{h}$ satisfy, respectively, (13) and (20), and $f_{i}(x, t, u), i = 1, 2$, satisfy (19). Then the nonlinear difference scheme (2) converges ε -uniformly to the solution of (1)

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

where U_i^* and u_i^* , i = 1, 2, are, respectively, the exact solutions to (2) and (1), C is a generic constant which is independent of ε , M_x and τ .

Proof Since the proof of the theorem follows the proof of Theorem 1 from [3], 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 integral-difference form (compare with (5) from [3])

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

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

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

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

$$T_{i}(x_{m}, t_{k}) = T_{i,1}(x_{m}, t_{k}) - I_{i}(x_{m}, t_{k}, u^{*}),$$
$$T_{i,1}(x_{m}, t_{k}) \equiv \frac{u_{i}^{*}(x_{m}, t_{k}) - u_{i}^{*}(x_{m}, t_{k-1})}{\tau_{k}} - \frac{\partial u_{i}^{*}(x_{m}, t_{k})}{\partial t}.$$

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

$$\|T_{i}(\cdot,t_{k})\|_{\omega^{h}} \leq \frac{1}{2} \max_{(x,t)\in Q} |u_{i,tt}^{*}|\tau_{k} + \|I_{i}(\cdot,t_{k})\|_{\omega^{h}}.$$
(22)

Thus, similar to [3], using bounds (18), 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], we prove the estimates

$$||I_i(\cdot, t_k)||_{\omega^h} \le C(M_x^{-1}\ln M_x), \quad i = 1, 2$$

From here and (22), we obtain

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

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) 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 starting from (15), where $-T_i$, i = 1, 2, are in use instead of \mathcal{R}_i , i = 1, 2, in (15).

Theorem 4 Assume that all the assumptions in Theorem 3 are satisfied. Then for the sequences $\{\overline{U}^{(n)}\}$ and $\{\underline{U}^{(n)}\}$, generated by (6), (11) with, respectively, $\overline{U}^{(0)} = \widetilde{U}$ and $\underline{U}^{(0)} = \widehat{U}$, the uniform in ε estimate holds

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

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).

Proof The proof of the theorem follows from Theorems 2 and 3.

5 Gas-Liquid Interaction Model

The gas-liquid interaction model in the non-dimensional variables can be presented in the form (see [4] 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 κ_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 ε 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) with $L_i = 1$, i = 1, 2, hold true. Thus, \widehat{U}_i and \widetilde{U}_i , i = 1, 2, from (17) are, respectively, lower and upper solutions to the test problem. From here, it follows that the inequalities in (12) 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 the error of the numerical solutions $U_i^{M_x}$, i = 1, 2, with respect to the reference 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). In Table 1, for parameters $\kappa_i = 1$, $i = 1, 2, t_{N_\tau} = 0.5, \tau = 5 \times 10^{-4}$ and different values of ε and M_x , we present 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 ε , has the first-order accuracy in the space variable, and the monotone sequences converge in few iterations.

M_{x}		32	64	128	256	512
$\varepsilon = 1$	E_{M_x}	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_x}	2	2	1	1	1
$\varepsilon = 10^{-1}$	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_x}	2	2	1	1	1
$\varepsilon = 10^{-2}$	E_{M_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	2	2	2
$\varepsilon = 10^{-3}$	E_{M_x}	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	2	2	2
$\varepsilon \le 10^{-4}$	E_{M_x}	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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