Appendix B. The Finite Difference Scheme

In this appendix we present numerical techniques which are used to approximate solutions of system (3.1)–(3.3). A comprehensive treatment of theoretical and implementation issues of discretization methods for advection-diffusion-reaction problems are given in the monograph by Hundsdorfer and Verwer Hundsdorfer, Verwer (2003). Very interesting applications of these results for biomedical problems are described by Gerisch and Chaplain Gerisch, Chaplan (2006), Gerisch and Verwer Gerisch, Verwer (2002) (see also references given in these publications).

Here we propose to use a linearized implicit backward Euler method for the approximation of the diffusion-reaction subproblems and the explicit forward Euler method for solution of the advection subproblem. We have restricted to the first order methods due to their robust stability. Note that our main goal is to investigate the influence of a possible ill-posedness of the PDE system to the asymptotical behaviour of the solution.

Appendix B.1. The method of lines. Discretization in space

We use the method of lines (MOL) approach (see, Gerisch, Chaplan (2006); Hundsdorfer, Verwer (2003)). At the first step we approximate the spatial derivatives in the PDE by applying robust and accurate approximations targeted for special physical processes described by differential equations.

Domain $[0,1]$ is covered by a discrete uniform grid

$$\omega_h = \{x_j : x_j = jh,\ j = 0, \dots, N-1\}, \quad x_N = 1$$

with the grid points x_j. On the semidiscrete domain $\omega_h(k) \times [0,T]$ we define functions $U_j(t) = U(x_j, t)$, $V_j(t) = V(x_j, t)$, $j = 0, \dots, N-1$, here U_j, V_j approximate solutions $u(x_j, t)$, $v(x_j, t)$ on the discrete grid ω_h at time moment t.

We also define the forward and backward space finite differences with respect to x:

$$\partial_x U_j = \frac{U_{j+1} - U_j}{h}, \quad \partial_{\bar{x}} U_j = \frac{U_j - U_{j-1}}{h}.$$

Using the finite volume approach, we approximate the diffusion and reaction terms in the PDE system (3.1) by the following finite difference equations:

$$A_{DR1}(U, j) = D\partial_{\bar{x}}\partial_x U_j + \gamma r U_j(1 - U_j), \tag{B.57}$$
$$A_{DR2}(V, U, j) = \partial_{\bar{x}}\partial_x V_j + \gamma \left(\frac{U_j^p}{1 + \beta U_j^p} - V_j \right).$$

The stencil of the discrete scheme requires to use functions defined outside of the grid ω_h. We apply periodicity boundary conditions (3.3) to define discrete functions for $j < 0$ or $j \geq N$:

$$U_{-j} = U_{N-j}, \quad U_{N-1+j} = U_{j-1} \quad \text{for} \ \ j > 0. \tag{B.58}$$

The advection term in equation (3.1) depends on the variable velocity

$$a(x, t) := \frac{\chi}{(1 + \alpha v)^2} \frac{\partial v}{\partial x},$$

therefore the maximum principle is not valid for the respective transport equation. But problem (3.1) still has non-negative solutions, and this property can be preserved on the discrete level by applying proper upwinding approximations. The discrete spatial approximation of the velocity is computed by

$$a_{j+\frac{1}{2}}(t) = \frac{\chi}{\big(1 + \alpha(V_j + V_{j+1})/2\big)^2}\, \partial_x V_j.$$

In the following we consider the upwind-based discrete fluxes Gerisch, Chaplan (2006); Hundsdorfer, Verwer (2003):

$$F_T(U, a, j + 1/2) = a_{j+\frac{1}{2}} \big[U_j + \psi(\theta_j)\big(U_{j+1} - U_j\big)\big], \quad a_{j+\frac{1}{2}} \geq 0, \tag{B.59}$$
$$F_T(U, a, j + 1/2) = a_{j+\frac{1}{2}} \big[U_{j+1} + \psi(1/\theta_{j+1})\big(U_j - U_{j+1}\big)\big], \quad a_{j+\frac{1}{2}} < 0,$$

with the Koren limiter function

$$\psi(\theta) = \max\Big(0, \min\big(1, \frac{1}{3} + \frac{1}{6}\theta, \theta\big)\Big).$$

The limiter ψ depends on the smoothness monitor function

$$\theta_j = \frac{U_j - U_{j-1}}{U_{j+1} - U_j}.$$

For $\psi = 0$ we get the standard first-order upwind flux

$$F_{TUW}(U, a, j + 1/2) = \max\left(a_{j+\frac{1}{2}}, 0\right) U_j + \min\left(a_{j+\frac{1}{2}}, 0\right) U_{j+1}.$$

Let us denote the discrete advection operator as

$$A_T(U, V, j) = \frac{1}{h}\big(F_T(U, a, j + 1/2) - F_T(U, a, j - 1/2)\big).$$

Then we obtain a nonlinear ODE system for the evaluation of the approximate semi-discrete solutions

$$\begin{aligned} \frac{dU_j}{dt} &= A_T(U, V, j) + A_{DR1}(U, j), \quad x_j \in \omega_h, \\ \frac{dV_j}{dt} &= A_{DR2}(V, U, j). \end{aligned} \tag{B.60}$$

Appendix B.2. Operator splitting methods

In order to develop efficient solvers in time for the obtained large ODE systems we apply the splitting techniques. They take into account the different nature of the discrete operators defining the advection $A_T(U, V, j)$ and the diffusion-reaction $A_{DR1}(U, j)$, $A_{DR2}(V, U, j)$ terms. The system resolving the semi-discrete advection process can be solved very efficiently by using explicit solvers, while the diffusion-reaction semi-discrete system is stiff and it requires an implicit treatment. Also we are interested in preserving at the discrete level the positivity and/or boundedness of the solution, if such properties hold for the differential ODE system.

First we consider the symmetrical splitting method (also known as the Strang splitting Strang (1968)). Given approximations U_j^n, V_j^n at time t^n, we compute solutions at $t^{n+1} = t^n + \tau$ by the following scheme:

$$\frac{dU_j}{dt} = A_T(U, V^n, j), \quad U_j(t^n) = U_j^n, \quad t^n \le t \le t^{n+\frac{1}{2}} = t^n + \tau/2, \tag{B.61}$$

$$\frac{dU_j}{dt} = A_{DR1}(U, j), \quad U_j(t^n) = U_j^{n+\frac{1}{2}}, \quad t^n \le t \le t^{n+1}, \tag{B.62}$$

$$\frac{dU_j}{dt} = A_T(U, V^n, j), \quad U_j(t^n) = U_j^{n+1}, \quad t^{n+\frac{1}{2}} \le t \le t^{n+1}$$

$$\frac{dV_j}{dt} = A_{DR2}(V, U, j), \quad V_j(t^n) = V_j^n, \quad t^n \le t \le t^{n+1}. \tag{B.63}$$

Here we also have splitted the given ODE system into two blocks with respect to U_j and V_j functions.

Lemma 1. *Solutions of the splitting ODE problem (B.61)–(B.63) are non-negative if* $U_j^n \ge 0$ *and* $V_j^n \ge 0$ *for all* $x_j \in \omega_h$.

Proof. The proof for the advection subsystems follows from the construction of the discrete fluxes by using the upwinding technique. The proof for the diffusion-reaction subsystems follows from the lemma in Gerisch, Verwer (2002) that the solution of an initial value problem for systems of ODEs

$$\frac{dY}{dt} = F(t, Y(t)), \quad t \ge 0, \quad Y(0) = Y_0$$

is non-negative if and only if for all t and any vector $V \in \mathbb{R}^m$ and all $1 \le i \le m$

$$v_i = 0, \;\; v_j \ge 0 \quad \text{for all} \;\; j \ne i \quad \Longrightarrow \quad f_i(t, V) \ge 0.$$

It is easy to see that for the diffusion-reaction subsystems the diffusion parts of the matrices are diagonally dominant and all off-diagonal entries are non-positive. For the reaction parts the required estimates are also trivially satisfied. □

Lemma 2. *If* $0 \le U_j^n \le C$ *for all* $x_j \in \omega_h$*, then a solution of the splitting ODE problem (B.62) is also bounded* $U_j \le \max(C, 1)$.

Proof. Here we use the fact that $U = 1$ is a stable attractor of the reaction function. Let $U_i^n = \max_j U_j^n$. Then it follows from the definition of $A_{DR1}(U, j)$ that in the worst case

$$\frac{dU_i}{dt} > 0, \;\; \text{if}\; C < 1, \qquad \frac{dU_i}{dt} = 0, \;\; \text{if}\; C = 1,$$

and

$$\frac{dU_i}{dt} < 0, \quad \text{if } C > 1.$$

The lemma is proved. □

Appendix B.3. Numerical integration of ODEs

There are many numerical integration methods for solution of non-stiff and stiff ODEs. For detailed discussions of these schemes we refer the reader to Gerisch, Chaplan (2006); Hairer, Norset, Wanner (1993); Hairer, Wanner (1996); Hundsdorfer, Verwer (2003).

Let ω_τ be a uniform time grid

$$\omega_\tau = \{t^n : t^n = n\tau, \, n = 0, \dots, M, \, M\tau = T_f\},$$

here τ is the time step. For simplicity this step size is taken constant.

In the following, we consider numerical approximations U_j^n, V_j^n to the exact solution values $u(x_j, t^n)$, $v(x_j, t^n)$ at the grid points $(x_j, t^n) \in \omega_h \times \omega_\tau$.

Remark 1. *In Baronas, Šimkus (2011), the explicit forward Euler scheme is used to solve problem (3.1). Since no details are given in Baronas, Šimkus (2011) on approximations of spatial derivatives, we use discrete operators introduced in previous sections and write the explicit forward Euler scheme as:*

$$\frac{U_j^{n+1} - U_j^n}{\tau} = A_T(U^n, V^n, j) + A_{DR1}(U^n, j),$$
$$\frac{V_j^{n+1} - V_j^n}{\tau} = A_{DR2}(V^n, U^n, j).$$

We note that this scheme can be written as a splitting algorithm:

$$\frac{U_j^{n+\frac{1}{2}} - U_j^n}{\tau} = A_T(U^n, V^n, j),$$
$$\frac{U_j^{n+1} - U_j^{n+\frac{1}{2}}}{\tau} = A_{DR1}(U^n, j),$$
$$\frac{V_j^{n+1} - V_j^n}{\tau} = A_{DR2}(V^n, U^n, j).$$

Thus the explicit Euler scheme can be considered as a special case of splitting algorithms. Despite easy implementation and good parallel properties of explicit algorithms, the main drawback of the explicit Euler method is that due to the conditional stability we must restrict the integration step to $\tau \leq Ch^2$ for stiff discrete diffusion-reaction subproblems.

The Rosenbrock and implicit Runge-Kutta methods are successfully applied for integration of a stiff part of the splitting semidiscrete-scheme, i.e. diffusion – reaction equations (B.62), (B.63), see Gerisch, Chaplan (2006); Gerisch, Verwer (2002); Hundsdorfer, Verwer (2003).

Here we propose to use a linearized implicit backward Euler method for the approximation of the diffusion-reaction subproblems and the explicit forward Euler method for solution of the advection subproblem. We have restricted to the first order methods due to their robust stability. Note that our main goal is to investigate the influence of a possible ill-posedness of the PDE system to the asymptotical behaviour of the solution.

We discretize the semidiscrete problem (B.61)–(B.63) with the fully discrete scheme

$$\frac{U_j^{n+\frac{1}{3}} - U_j^n}{0.5\tau} = A_T(U^n, V^n, j), \tag{B.64}$$

$$\frac{U_j^{n+\frac{2}{3}} - U_j^{n+\frac{1}{3}}}{\tau} = D\partial_{\bar{x}}\partial_x U_j^{n+\frac{2}{3}} + \gamma r U_j^{n+\frac{1}{3}}\left(1 - U_j^{n+\frac{2}{3}}\right), \tag{B.65}$$

$$\frac{U_j^{n+1} - U_j^{n+\frac{2}{3}}}{0.5\tau} = A_T(U^{n+\frac{2}{3}}, V^n, j), \tag{B.66}$$

$$\frac{V_j^{n+1} - V_j^n}{\tau} = A_{DR2}(V^{n+1}, U^{n+1}, j). \tag{B.67}$$

We apply two splittings of the advection term, because then we use only half of the splitting step size for the explicit method. This doubles the stability and positivity domains of the explicit method (see Gerisch, Verwer (2002)).

Next we prove that statements of Lemma 1 and 2 hold also for solutions of the fully discrete finite difference scheme (B.64)–(B.67)

Lemma 3. *For a sufficiently small time step $\tau \leq \tau_0$ solutions of the finite difference scheme (B.64)–(B.67) are non-negative if $U_j^n \geq 0$ and $V_j^n \geq 0$ for all $x_j \in \omega_h$.*

Proof. The proof for the advection problems (B.64) and (B.66) follows from the construction of the discrete fluxes by using the upwinding technique and selection of a sufficiently small time step $\tau \leq \tau_0$.

The proof for the diffusion-reaction problems (B.65) and (B.67) follows from the maximum principle Samarskii (2001). For example, consider problem (B.65). We assume, that

$$U_i^{n+\frac{2}{3}} = \min_{0 \leq j < N} U_j^{n+\frac{2}{3}}.$$

We write the discrete equation (B.65) for $U_i^{n+\frac{2}{3}}$ in an explicit form

$$\left(1+\tau\gamma r U_i^{n+\frac{1}{3}}\right) U_i^{n+\frac{2}{3}} = \left(1+\tau\gamma r\right) U_i^{n+\frac{1}{3}} + \frac{D\tau}{h^2}\left(U_{i+1}^{n+\frac{2}{3}} + U_{i-1}^{n+\frac{2}{3}} - 2U_i^{n+\frac{2}{3}}\right)$$

Since $U_i^{n+\frac{1}{3}} \geq 0$ and $U_{i\pm 1}^{n+\frac{2}{3}} \geq U_i^{n+\frac{2}{3}}$ we get that $U_i^{n+\frac{2}{3}} \geq 0$. □

Lemma 4. *If $0 \leq U_j^{n+\frac{1}{3}} \leq C$ for all $x_j \in \omega_h$, then a solution of the finite difference scheme (B.65) is also bounded*

$$U_j^{n+\frac{2}{3}} \leq \max(C, 1), \quad \forall x_j \in \omega_h.$$

Proof. The proof is based on the maximum principle and a special form of the discrete reaction term. First, we consider the case $C \leq 1$. Let $U_i^{n+\frac{2}{3}} = \max_j U_j^{n+\frac{2}{3}}$. Then it follows from (B.65) that

$$\left(1+\tau\gamma r U_i^{n+\frac{1}{3}}\right) U_i^{n+\frac{2}{3}} \leq \left(1+\tau\gamma r\right) U_i^{n+\frac{1}{3}} \implies U_i^{n+\frac{2}{3}} \leq \frac{(1+\tau\gamma r) U_i^{n+\frac{1}{3}}}{1+\tau\gamma r U_i^{n+\frac{1}{3}}} \leq 1.$$

Next we consider the case $C > 1$. Then we get that

$$U_i^{n+\frac{2}{3}} \leq \frac{(1+\tau\gamma r) U_i^{n+\frac{1}{3}}}{1+\tau\gamma r U_i^{n+\frac{1}{3}}} = 1 + \frac{U_i^{n+\frac{1}{3}} - 1}{1+\tau\gamma r U_i^{n+\frac{1}{3}}} < C.$$

The lemma is proved. □