Propagator Method for Numerical Solution of the Cauchy Problem for ADR Equation

J.Rimšāns and D.Žaime

Summary. A new numerical scheme based on our propagator method is presented for solution of ADR equations. The method exploits an approach of a non-standard representation of the time derivative, by applying the derivative to the solution given as the product of two functions, where one of them is a propagator function. Propagator function is chosen in nonlocal way, and with respect to the solution, a new finite volume difference scheme is presented. Stability of the scheme is investigated. It is shown, that stability restrictions for the propagator scheme become more weaker in comparison to traditional semi-implicit difference schemes. There are some regions of ADR coefficients, for which elaborated propagator difference scheme becomes absolutely stable. It is proven that the scheme is unconditionally monotonic. The scheme has the first order in time and the second order truncation errors in space. The scheme can be easy extended to the solution of multidimensional non-steady problems.

MSC 35K15, 35K57, 65N06, 65N12

1 Introduction

Advective dispersive reactive (ADR) equation [1] is a model of a problem that incorporates with the diffusive, bulk solute movement and sorptive processes. The Cauchy problem for non-steady ADR equation is given as follows:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + f(\frac{\partial c}{\partial x}, c), \quad f = -R_e v \frac{\partial c}{\partial x} - kc, \quad x \in \Re, \tag{1}$$

$$c(0, x) = c_0(x). \tag{2}$$

The ADR equation (1) is written in a normalized form $c = \hat{c}/c^*$, $v = \hat{v}/U$, $t = \hat{t}/T$, $x = \hat{x}/L$, by using normalization coefficients $c^* = 1m^{-3}$, $T = L^2/\hat{D}$, R_e is the Reynolds number $R_e = UL/\hat{D}$, and $k = \hat{\lambda}L^2/\hat{D} \geq 0$, $\hat{v} = \hat{u}/R$, where $R > 0$ is a factor of retardation, $\hat{D} \geq d > 0$ is a diffusion coefficient, $\hat{D} = \hat{v}\hat{\alpha}$, $\hat{\alpha}$ is longitudinal groundwater dispersivity, $\hat{c}$ is concentration of chemical components, $\hat{u}$ is contaminant velocity, $\hat{\lambda} = \hat{k}/R$, $\hat{k} \geq 0$ is hydraulic conductivity and L is a length of region.

In recent years a modern geochemical transport models have become more and more complex. Problem (1)-(2) is the simplest way to describe such phenomena, and for them is at least the particular analytical solution [2]. Although a general solution of the problem usually can be represented as the result of infinity sum. The summation can cause specific difficulties, and numerical solution of the problem (1)-(2) is a likelihood to existing others. Moreover, as our elaborated method can easily be extended for solution of general ADR problems, we look at equation (1) in order to treat numerical method.

Numerical methods for solving advective-diffusive-reactive equations are investigated and described in [1], [4] -[6], [8]. The application of known numerical solution methods usually has computational difficulties related with restrictions on the time step caused by numerical instability. Traditionally, there are two approaches: explicit and implicit approach for numerical solution of non-steady state problems.

In [5] modern geochemical transport models are described, the implicit difference scheme by applying splitting for chemical reaction and transport operators for solving of equations is used. Scheme is absolutely stable, designed with rather extremely fine grids to account small-scale characteristics. It requires extreme memory for keeping of matrixes, and special algorithms for finding inverse matrix should be used, which cause a growth of computer calculations and require use of parallel computations. In this case, to fully exploit the advanced computing power of today's supercomputers, innovative algorithms have to be developed.

In [8] wide theoretical investigations for numerical solving second order elliptic and parabolic equations are provided. The advantages of explicit/implicit methods of numerical solution are described, including the semi-implicit case, when the inverse matrix can be easily calculated and stability restrictions are not so hard as for explicit methods. Stability conditions for convection-diffusion equations are investigated by applying ϱ (regular stability) criterion.

We offer a new semi-implicit propagator difference scheme for solving ADR equations. By applying von Neumann's strict stability criterion and using Cauchy problem analytical solution (estimation) improvement for stability limits of our proposed difference scheme is shown.

In our consideration we introduce a non-regular grid $\overline{\omega} = \overline{\omega}_h \times \overline{\omega}_\tau$:

$$\begin{aligned}
&\overline{\omega}_h = \{x_i,\ i = 0, 1, 2, ..., N,\ x_0 = 0,\ x_N = L\},\ \overline{\omega}_\tau = \{t_l,\ l = 0, 1, 2, ..., M; \\
&t_0 = 0,\ t_M = T\}, \\
&x_i > x_{i-1},\ h_i = x_i - x_{i-1},\ i = 1, 2, 3, ..., N;\ t_l > t_{l-1},\ t_l = t_l - t_{l-1}, \\
&l = 1, 2, 3, ..., M,
\end{aligned}$$

where h and τ are space and time steps, respectively.

In order to describe our approach in the next section we analyze stability features of the semi-implicit central difference scheme.

2 Stability analysis for the central difference scheme

For stability analysis we consider the square quasi-uniform mesh, with $x_i = ih, \quad i = 0, 1, 2, ..., N,\ x_N = L,\ t_l = l\tau,\ l = 0, 1, 2, ..., M,\ t_M = T$.

For a function C defined on $\overline{\omega}_{\tau,h} = \overline{\omega}_\tau \times \overline{\omega}_h$ let us assume that:

$$\begin{aligned}
&C_i^l = C(t_l, x_i), \quad \partial_t C^l(x) = \tau^{-1}\left(C(t_{l+1}, x) - C(t_l, x)\right),\\
&\partial_x C^l(x) = h^{-1}\left(C(t_l, x+h) - C(t_l, x)\right),\\
&\overline{\partial}_x C^l(x) = h^{-1}\left(C(t_l, x) - C(t_l, x-h)\right).
\end{aligned} \tag{3}$$

The semi-implicit central difference scheme for solving equation (1) is:

$$\partial_t C^l(x) = \Delta^h C^{l+1}(x) - R_e v \frac{1}{2h}\left(C^l(x+h) - C^l(x-h)\right) - kC^l(x), \tag{4}$$

$$\Delta^h C^l(x) = \partial_x \overline{\partial}_x C^l(x). \tag{5}$$

The solution of the difference scheme (4) will be expressed in the form:

$$C^l(x) = \tilde{C}^l(x) + \delta C^l(x), \tag{6}$$

where $\tilde{C}^l$ is an unperturbed solution of the difference scheme (4) and δC^l is a perturbation on the time step l.

After substitution of solution (6) in the difference scheme (4), we can write equation for them:

$$\frac{\delta C_i^{l+1} - \delta C_i^l}{\tau} = \frac{1}{h^2}(\delta C_{i+1}^{l+1} - 2\delta C_i^{l+1} + \delta C_{i-1}^{l+1}) - R_e v \frac{\delta C_{i+1}^l - \delta C_{i-1}^l}{2h} - k\delta C_i^l. \tag{7}$$

By using von Neumann approach we introduce substitution $\delta C_i^l = (G^*)^l \exp(Ii\varphi)$, as a result, expression for G^* from (7) is obtained:

$$G^* = \frac{[\frac{1}{\tau} - \frac{R_e v}{2h}(\exp(I\varphi) - \exp(-I\varphi)) - k]}{\frac{1}{\tau} - \frac{1}{h^2}(\exp(I\varphi) - 2 + \exp(-I\varphi))}, \tag{8}$$

and writing $\exp(I\varphi) = \cos\varphi + I\sin\varphi$, from (8), we get

$$G = \frac{\sqrt{(1-k\tau)^2 + \frac{R_e^2 v^2 \tau^2}{h^2}\sin^2\varphi}}{\sqrt{(1 + \frac{4\tau}{h^2}\sin^2\frac{\varphi}{2})^2}}, \tag{9}$$

where $G = |G^*|$. The stability condition for equation (7) is $G \le 1$. In order to fulfill the stability condition, and by introducing a notation:

$$\mu = \frac{\tau}{h^2}, \quad s = sin^2\frac{\varphi}{2}, \quad 0 \le s \le 1, \tag{10}$$

such inequality follows:

$$-1 \le \frac{(1-k\mu h^2)^2 + 4\frac{R_e^2 v^2 \mu^2 h^4}{h^2} s(1-s)}{(1+4\mu s)^2} \le 1. \tag{11}$$

Solution for the left side of inequality (11) is obviously true for all values of μ, because both counter and denominator always are positive. The right side of inequality (11) gives:

$$\mu(k^2h^4 + 4R_e^2v^2h^2s(1-s) - 16s^2) - (2kh^2 + 8s) \leq 0. \tag{12}$$

Considering inequality (12), it follows that second term always is positive, and if for each s fulfills

$$k^2h^4 + 4R_e^2v^2h^2s(1-s) - 16s^2 \leq 0, \tag{13}$$

then inequality (12) is true for all values of μ and the semi-implicit difference scheme (4) should be absolutely stable. Although it is worth to mention that it happens for all s only when $k = 0$ and $v = 0$, or when equation (1) is a diffusion equation, for which, as it is known, semi-implicit central difference scheme is absolutely stable [4]. In all other cases when $k \neq 0$ or $v \neq 0$ there are some s values $s \in [0, s_0)$, where

$$s_0 = \frac{R_e^2v^2h^2 + h^2\sqrt{R_e^4v^4 + 4k^2 + R_e^2v^2h^2k^2}}{2(4 + R_e^2v^2h^2)}, \tag{14}$$

for which inequality (13) does not fulfill. As it follows from expression (14) s_0 lies in interval $s_0 \in (0, \infty)$. For these cases we should solve inequality (12) in respect to μ. That means semi-implicit central difference scheme (4) for the ADR equation (1) is only conditionally stable.

Let us introduce such notation

$$a = R_e^2v^2h^2, \quad b = kh^2. \tag{15}$$

Then we obtain such restriction from (12) for μ , where $s \in [0, s_0)$:

$$\mu \leq \mu_0(s) = \frac{2b + 8s}{b^2 + 4as(1-s) - 16s^2}, \tag{16}$$

where, as we assumed $b^2 + 4as(1-s) - 16s^2 > 0$. By using MATHEMATICA® in order to obtain the maximal allowed μ for each a and b we find extremum s_0^*:

$$s_0^* = \frac{-4b - ab + \sqrt{16ab + 4a^2b + 4ab^2 + a^2b^2}}{4(4+a)}, \tag{17}$$

for which the right side of inequality (16) reaches the minimum.

It should be noted that extremum s_0^* lies in the interval $s_0^* \in (-\infty, \frac{1}{2}]$, when $a \in [0, \infty)$ and $b \in [0, \infty)$, which is partially out of the allowed values for s:

$$s \in [0, s_0), \quad if \quad s_0 < 1, \tag{18}$$

$$s \in [0, 1], \quad if \quad s_0 \geq 1. \tag{19}$$

Depending on s_0^*, for different values of a and b we will obtain two criterions limiting maximal τ. One of them follows for s_0^* values $s_0^* \in (-\infty, 0)$, and the next one for $s_0^* \in [0, \frac{1}{2}]$.

At first we will look at s_0^* in the interval $s_0^* \in (-\infty, 0)$. In this case extremum s_0^* is out of the allowed values (18) or (19). Limiting τ should be found from $\min\{\mu_0(0), \mu_0(s_0)\}$ or $\min\{\mu_0(0), \mu_0(s_0),\}$ depending on (18)-(19). It can be shown that $\mu_0(0) < \mu_0(1)$ and $\mu_0(0) < \mu_0(s_0)$. Namely, we have negative signs in the following expressions:

$$\mu_0(0) - \mu_0(1) = -\frac{(8b + 32)}{(b^2 - 16)b}, \tag{20}$$

$$\mu_0(0) - \mu_0(s_0) < 0, \tag{21}$$

where the denominator of expression (20) is positive, as follows from the definition of $\mu_0(s)$ in (16), and inequality (21) fulfills, because:

$$\lim_{s \to s_0} \mu_0(s) \to \infty. \tag{22}$$

So, right side of (16) is minimal, when limit value $s = 0$ will be substituted in it, i.e. $\mu_0 = \mu_0\,(0)$. Moreover, taking into account (22), values of $\mu_0(s)$, when $s \to s_0$, will be omitted as a restriction for τ in further consideration.

Then, in respect to the expression (10) for μ, the stability condition for semi-implicit central difference scheme for ADR equation from (16) may be written in a form:

$$\tau \le \frac{2}{k}. \tag{23}$$

The obtained inequality (23) for limiting τ is also true for the special case for diffusion reaction equation, when $v = 0$, $k \ne 0$, because in this case $s_0^* = -\frac{b}{4} < 0$.

Secondly, we consider s_0^* from the interval $s_0^* \in [0, \frac{1}{2}]$. In this case requiring in addition $s_0 > \frac{1}{2}$, after s is substituted by the extremum s_0^* in the right side of inequality (16), for all values of v and k in respect to expressions for a and b from (15) for semi-implicit central difference scheme we obtain the following limiting τ:

$$\begin{aligned} &\tau \le h^2 \min\{\mu_0(0), \mu_0(s_0^*)\} = \\ &\min\{\frac{2}{k}, \frac{4}{4k + R_e^2 v^2(2 + kh^2) - R_e v\sqrt{k(4 + kh^2)(4 + R_e^2 v^2 h^2)}}\}. \end{aligned} \tag{24}$$

In the case $s_0 \in (0, \frac{1}{2}]$ and $s_0^* > s_0$ we obtain stability condition (23) by substituting $s = 0$ in the right side of inequality (16) for μ. When $s_0 \in (0, \frac{1}{2}]$ and $s_0^* \in [0, s_0)$ we obtain stability condition (24) again.

In a special case for advection diffusion equation, when $k = 0$, $v \ne 0$, we obtain from (24):

$$\tau \le \frac{2}{R_e^2 v^2}. \tag{25}$$

Inequalities (23), (24), and (25) are stability conditions for the semi-implicit difference scheme, when at least one of the coefficients k and v are not equal to zero.

3 Propagator difference scheme

In our propagator method solution is represented as multiplication of two functions

$$c = \eta\left(t, x\right) g\left(t, x\right), \tag{26}$$

where propagator function η is chosen in nonlocal way:

$$\eta = \eta_0 + \int_0^t \frac{f}{c}\eta dt, \quad \eta_0 = const. \tag{27}$$

It can be written

$$\eta = \sum_{n=0}^{l} \eta_n + \int_{t_l}^{t} \frac{f}{c}\eta dt, \quad \eta_n = \int_{t_n}^{t_{n+1}} \frac{f}{c}\eta dt, \tag{28}$$

and assuming, that $\frac{f}{c} = const$, $t \in [t_l,\ t_{l+1}]$, $l = 0, 1, 2, ..., M-1$, we have:

$$\eta = \sum_{n=0}^{l} \eta_n + \frac{f}{c}\int_{t_l}^{t} \eta dt. \tag{29}$$

The solution of equation (29) is:

$$\eta = \eta_i^l exp\left(\frac{f_i^{l+1}}{c_i^{l+1}}(t - t_l)\right), \quad \eta_i^l = exp\left(\sum_{n=0}^{l} \frac{f_i^n}{c_i^n}\tau_n\right). \tag{30}$$

Substituting the obtained expression (30) for $\eta(t, x)$ in (26) we get:

$$c = \eta_i^l exp\left(\frac{f_i^{l+1}}{c_i^{l+1}}(t - t_l)\right) g\left(t, x\right). \tag{31}$$

As a result, taking into account new expression (31) for c the equation (1) can be written:

$$\eta\frac{\partial g}{\partial t} = \frac{\partial^2}{\partial x^2}(\eta g). \tag{32}$$

By applying integro-interpolation method [9] a difference scheme for the equation (32) can be obtained in such form:

$$\begin{aligned} &\eta_i^{l+1}\frac{g_i^{l+1} - g_i^l}{\tau_{l+1}} = \frac{1}{h_i^*}\left(\frac{C_{i+1}^{l+1} - C_i^{l+1}}{h_{i+1}} - \frac{C_i^{l+1} - C_{i-1}^{l+1}}{h_i}\right), \\ &h_i^* = \frac{1}{2}\left(h_i + h_{i+1}\right), \end{aligned} \tag{33}$$

or

$$\frac{1}{h_i^* h_{i+1}}C_{i+1}^{l+1} + \frac{1}{h_i^* h_i}C_{i-1}^{l+1} - \left(\frac{1}{h_i^*}\left(\frac{1}{h_{i+1}} + \frac{1}{h_i}\right) + \frac{1}{\tau_{l+1}}\right)C_i^{l+1} = -\frac{\eta_i^{l+1}}{\eta_i^l}\frac{C_i^l}{\tau_{l+1}}. \tag{34}$$

Equation (34) can be written in a simple way, taking into account $\frac{\eta_i^{l+1}}{\eta_i^l} = exp\left(\frac{f_i^{l+1}}{C_i^{l+1}}\tau_{l+1}\right)$.

As a result, a new fully implicit propagator difference scheme for equation (32) in respect to unknown C can be written in a final form:

$$\Lambda\left(C^{l+1,m+1}\right)_i = \frac{1}{h_i^*}B_i C_{i+1}^{l+1,m+1} + \frac{1}{h_i^*}A_i C_{i-1}^{l+1,m+1} - Q_i C_i^{l+1,m+1} =$$
$$-exp\left(\frac{f_i^{l+1,m}}{C_i^{l+1,m}}\tau_{l+1}\right)\frac{C_i^l}{\tau_{l+1}}, \quad 1 \le i \le N-1, \quad 1 \le l \le M-1 \tag{35}$$

where

$$f_i^{l+1,m} = -R_e v \frac{C_{i+1}^{l+1,m} - C_{i-1}^{l+1,m}}{2h_i^*} - kC_i^{l+1,m}, \tag{36}$$

$$A_i = \frac{1}{h_i}, \quad B_i = \frac{1}{h_{i+1}}, \quad Q_i = \frac{1}{h_i^*}\left(A_{i+1} + B_{i-1}\right) + \frac{1}{\tau_{l+1}}, \tag{37}$$

and $m = 1, 2, 3, ...$ is an iteration index.

Finally, by assuming that $(c_0)_i \ge 0$ for the initial condition (2), it can be concluded that the difference scheme (35)-(37) is unconditionally monotone, since the coefficients (37) of this scheme satisfy the maximal principle conditions [7], which are formulated as follows.

Lemma 1 *Let $(c_0)_i \ge 0$, $i = 0, 1, 2, ..., N$ then it follows that $C_i^{l,m}$ cannot assume a minimum value that is negative at any of the nodes $0 \le i \le N$ for each time step $0 \le l \le M$ on the iteration m. That is $C_i^{l,m} \ge 0$, because [7]*

$$\Lambda\left(C^{l+1,m+1}\right)_i \le 0, \quad A_i > 0, \quad B_i > 0, \tag{38}$$

and

$$Q_i = \frac{1}{h_i^*}\left(A_{i+1} + B_{i-1}\right) + \Xi, \quad \Xi = \frac{1}{\tau_{l+1}} \ge 0. \tag{39}$$

To study the consistency, using specific non-regular grid $\overline{\omega}$, with $\tau_1 = \tau$, and

$$\frac{\tau_{l+1}}{\tau_l} = (1 \pm o), \quad o > 0, \quad o \to 0, \tag{40}$$

for $h_1 = h$, and

$$\frac{h_{i+1}}{h_i} = (1 \pm q), \quad q > 0, \quad q \to 0, \tag{41}$$

we examine the Taylor expansions of the C and f in the vicinity of the time and space grid point (t_l, x_i). It can be shown that the semi-implicit propagator central difference scheme $(35)-(37)$ has a maximum first order truncation error in time and a second order truncation error in space $O\left(o + \tau + q + qh + h^2\right)$.

4 Stability of the semi-implicit propagator difference scheme

In the further consideration we will look only at semi-implicit difference scheme, which can be obtained from (35) by assuming that the right side expression depends only from the time on l level. Then, omitting iteration index m in (35), semi-implicit propagator difference scheme with the same coefficients A_i, B_i, and Q_i as in (37) can be written as follows:

$$\Lambda\left(C^{l+1}\right)_i = \frac{1}{h_i^*}B_iC_{i+1}^{l+1} + \frac{1}{h_i^*}A_iC_{i-1}^{l+1} - Q_iC_i^{l+1} =$$
$$-exp\left(\frac{f_i^l}{C_i^l}\tau_l\right)\frac{C_i^l}{\tau_{l+1}}, \quad 1 \le i \le N-1, \quad 1 \le l \le M-1, \tag{42}$$

with

$$f_i^l = -R_e v\frac{C_{i+1}^l - C_{i-1}^l}{2h_i^*} - kC_i^l. \tag{43}$$

To find a stability for the semi-implicit propagator difference scheme (42) – (43) we will express solution of the scheme and forcing term in the form:

$$C^l(x) = \tilde{C}^l(x) + \delta C^l(x), \quad f^l(x) = \tilde{f}^l(x) + \delta f^l(x), \tag{44}$$

where

$$\delta f = \frac{\partial\tilde{f}}{\partial\tilde{C}_{i+1}}\delta C_{i+1} + \frac{\partial\tilde{f}}{\partial\tilde{C}_i}\delta C_i + \frac{\partial\tilde{f}}{\partial\tilde{C}_{i-1}}\delta C_{i-1}. \tag{45}$$

In the expressions (44) $\tilde{C}$ is solution of difference scheme or estimation of the solution and $\tilde{f}$ is the forcing term depending on $\tilde{C}$. As such $\tilde{C}$ estimation we will use known particular analytical Domenico solution c_d of the problem (1) – (2) from [2], [3]:

$$c_d = \frac{C_0}{8}e^{-\frac{1}{2}R_e\left(-1+\sqrt{1+\frac{4k}{R_e^2v^2}}\right)\cdot v\cdot x}\cdot erfc\left(\frac{-R_e\cdot t\cdot v\sqrt{1+\frac{4k}{R_e^2\cdot v^2}}+x}{2\sqrt{t}}\right). \tag{46}$$

By assuming $\tilde{C} = c_d$ and using expressions (44), we have for the Taylor expansion of the right side expression of equation (42):

$$exp\left(\frac{f_i}{C_i}\tau\right)\frac{C_i}{\tau} = \left(\tilde{f}_i + \frac{(c_d)_i}{\tau} + \frac{\tilde{f}_i^2\tau}{2(c_d)_i}\right) + \left(\frac{\partial\tilde{f}_i}{\partial\tilde{C}_{i+1}} + \frac{\partial\tilde{f}_i}{\partial\tilde{C}_{i+1}}\cdot\frac{\tilde{f}_i\tau}{(c_d)_i}\right)\cdot\delta C_{i+1}$$
$$+\left(\frac{\partial\tilde{f}_i}{\partial\tilde{C}_i} + \frac{1}{\tau} + \frac{\partial\tilde{f}_i}{\partial\tilde{C}_i}\cdot\frac{\tilde{f}_i\tau}{(c_d)_i} - \frac{\tilde{f}_i^2\tau}{2(c_d)_i^2}\right)\cdot\delta C_i$$
$$+\left(\frac{\partial\tilde{f}_i}{\partial\tilde{C}_{i-1}} + \frac{\partial\tilde{f}_i}{\partial\tilde{C}_{i-1}}\cdot\frac{\tilde{f}_i\tau}{(c_d)_i}\right)\cdot\delta C_{i-1} + O(\tau^2). \tag{47}$$

To make c_d the solution of the difference scheme $(42)-(43)$ we require that the regular term $\frac{\tilde{f}_i^2\tau}{2(c_d)_i}$ in the first bracket of the expression (47) should be small in respect to the forcing term $\mid \tilde{f}_i \mid$:

$$\frac{\tilde{f}_i^2\tau}{2(c_d)_i} \ll \mid \tilde{f}_i \mid, \quad or \quad \left|\frac{\tilde{f}_i\tau}{2(c_d)_i}\right| \ll 1. \tag{48}$$

By taking into account the estimation (48) and as a result, omitting small summands of the right side of (47) , i.e. the third summand from the first and third brackets, the second summand from the second and fourth brackets, and keeping only first order terms in respect to τ we obtain:

$$exp\left(\frac{f_i}{C_i}\tau\right)\frac{C_i}{\tau} = \left(\tilde{f}_i + \frac{(c_d)_i}{\tau}\right) + \frac{\partial \tilde{f}_i}{\partial \tilde{C}_{i+1}}\cdot \delta C_{i+1} + \\ + \left(\frac{\partial \tilde{f}_i}{\partial \tilde{C}_i} + \frac{1}{\tau} - \frac{\tilde{f}_i^2\tau}{2(c_d)_i^2}\right)\cdot \delta C_i + \frac{\partial \tilde{f}_i}{\partial \tilde{C}_{i-1}}\cdot \delta C_{i-1}. \tag{49}$$

By taking into account expression (49) for the right side of difference scheme (42) we have a difference scheme for the perturbations δC:

$$\frac{1}{h_i^*}B_i\delta C_{i+1}^{l+1} + \frac{1}{h_i^*}A_i\delta C_{i-1}^{l+1} - Q_i\delta C_i^{l+1} = -\frac{\partial \tilde{f}_i^l}{\partial \tilde{C}_{i+1}^l}\cdot \delta C_{i+1}^l + \\ \left(-\frac{\partial \tilde{f}_i^l}{\partial \tilde{C}_i^l} - \frac{1}{\tau} + \tilde{F}_i^l\tau\right)\cdot \delta C_i^l - \frac{\partial \tilde{f}_i^l}{\partial \tilde{C}_{i-1}^l}\cdot \delta C_{i-1}^l, \tag{50}$$

where $\tilde{F}_i^l = \frac{1}{2}\left(\frac{\tilde{f}_i^l}{(c_d)_i^l}\right)^2$. By using the analytical Domenico solution (46) the function $\tilde{F}$ is:

$$\tilde{F} = \frac{e^{\tilde{F}_1}\left(2R_e v + e^{\tilde{F}_2}\sqrt{\pi t}\tilde{F}_3\cdot erfc(\tilde{F}_4)\right)^2}{8\pi t\cdot erfc^2(\tilde{F}_4)}. \tag{51}$$

For large positive $\tilde{F}_4$ values, to avoid division by zero in (51), we use asymptotic expression [10] for $erfc$ and obtain such final form for function $\tilde{F}$:

$$\tilde{F} = \frac{\left(\frac{2R_e v\tilde{F}_4}{1+\tilde{F}_5}\cdot e^{\frac{\tilde{F}_1}{2}+\tilde{F}_4^2} + \sqrt{t}\cdot\tilde{F}_3\cdot e^{\frac{\tilde{F}_1}{2}+\tilde{F}_2}\right)^2}{8t}, \tag{52}$$

where

$$\tilde{F}_1 = -\frac{1}{2}\left(4kt + R_e^2tv^2 - 2R_evx\sqrt{1+\frac{4k}{R_e^2v^2}} + \frac{x^2}{t}\right),$$

$$\tilde{F}_2 = \frac{\left(x - R_evt\sqrt{1+\frac{4k}{R_e^2v^2}}\right)^2}{4t}, \quad \tilde{F}_3 = R_e^2v^2\cdot\left(\sqrt{1+\frac{4k}{R_e^2v^2}} - 1\right) - 2k,$$

$$\tilde{F}_4 = \frac{x - R_evt\cdot\sqrt{1+\frac{4k}{R_e^2v^2}}}{2\sqrt{t}}, \quad \tilde{F}_5 = \sum_{m=1}^{\infty}(-1)^m\frac{1\cdot 3\cdot \ldots \cdot(2m-1)}{(2\tilde{F}_4)^m}. \tag{53}$$

Now, using for the propagator difference scheme the analogous method as for the central difference scheme, for G we obtain:

$$G = \frac{\sqrt{(1 - k\tau - F\tau^2)^2 + \frac{R_e^2 v^2 \tau^2}{h^2}\sin^2\varphi}}{\sqrt{(1 + \frac{4\tau}{h^2}\sin^2\frac{\varphi}{2})^2}}, \quad F = \min_{0<i<N} \tilde{F}_i^l. \tag{54}$$

From (54) follows the stability condition for μ:

$$\mu(k^2h^4 - 2Fh^4 + 4R_e^2v^2h^2s(1-s) - 16s^2) - (2kh^2 + 8s) + O(\tau^2) \leq 0. \tag{55}$$

In order to find stability conditions we will look at each term in the inequality (55). Firstly, we omit second order term in respect to τ, considering it is small in comparison to others. The second term is always positive and we will look only at the first term in this inequality.

4.1 The case of absolute stability for the propagator difference scheme

The first term in inequality (55) is required to be negative. To fulfill this we rewrite the first term of inequality (55) in such notation $\mu\Upsilon(s)$, where

$$\Upsilon(s) = k^2h^4 - 2Fh^4 + 4R_e^2v^2h^2s(1-s) - 16s^2. \tag{56}$$

Taking into account that μ is always positive we will require that:

$$\Upsilon(s) \leq 0. \tag{57}$$

Then, if (57) fulfills, inequality (55) is true for all values of μ and the propagator difference scheme (42) is absolutely stable.

It should be noted, that $\Upsilon(s)$ reaches the maximum in respect to s, when $s = s_{max}$, where $s_{max} = (R_e^2v^2h^2)\,/\,(2R_e^2v^2h^2 + 8)$. If inequality (57) fulfills for s_{max}, the propagator difference scheme is always stable. By inserting s_{max} into (57) we get absolute stability condition for the propagator difference scheme:

$$F \geq \frac{8}{h^4(4 + R_e^2v^2h^2)} + \frac{k^2h^2 + R_e^2v^2}{2h^2} - \frac{2}{h^4}. \tag{58}$$

In comparison to the central difference scheme the propagator difference scheme for some region of parameters R_e, k and v shows absolute stability features, when (58) fulfills.

4.2 Time step restrictions for the propagator difference scheme

In case, when condition (58) does not fulfill and $\Upsilon(s) > 0$, there are some s values $s \in [0, s_f)$, where:

$$s_f = \frac{R_e^2v^2h^2 + h^2\sqrt{R_e^4v^4 + 4k^2 + R_e^2v^2h^2k^2 - 8F - 2R_e^2v^2h^2F}}{2(4 + R_e^2v^2h^2)}, \tag{59}$$

for which we should solve inequality (55) in respect to μ in order to find stability conditions. As it follows from (59), in case when $k \neq 0$ or $v \neq 0$, s_f lies in the interval $s_f \in [0, \infty)$, because, if (58) does not fulfill, the subduplicate expression in (59) is positive. In respect to values of a and b from (15), for μ we obtain such restriction:

$$\mu \leq \mu_f(s) = \frac{2b + 8s}{b^2 - 2Fh^4 + 4as(1-s) - 16s^2}, \tag{60}$$

where $\Upsilon(s) = b^2 - 2Fh^4 + 4as(1-s) - 16s^2 > 0$ and $s \in [0, s_f)$. In order to obtain maximal allowed μ by using MATHEMATICA® for each a and b we find extremum s_f^*:

$$s_f^* = \frac{-4b - ab + \sqrt{16ab + 4a^2b + 4ab^2 + a^2b^2 + 32Fh^4 + 8aFh^4}}{4(4+a)}, \tag{61}$$

for which the right side of inequality (60) reaches the minimum.

For each $a \in [0, \infty)$ and each $b \in [0, \infty)$ it is true, that extremum $s_f^* \in (-\infty, \infty)$ is partially out of the allowed values of s:

$$s \in [0, s_f), \quad if \quad s_f < 1, \tag{62}$$

$$s \in [0, 1], \quad if \quad s_f \geq 1. \tag{63}$$

As in stability conditions for semi-implicit difference scheme we obtain two criterions limiting maximal τ.

One of them follows for s_f^* values $s_f^* \in (-\infty, 0)$. Extremum s_f^* is out of the allowed values at (62) or (63). Limiting τ should be found as $\min\{\mu_f(0), \mu_f(s_f)\}$ or $\min\{\mu_f(0), \mu_f(1)\}$. As in the case for central difference scheme the value of $\mu_f(s)$, when $s \to s_f$, will be omitted. It can be shown that $\mu_f(0) - \mu_f(1) < 0$ for all allowed values of F, when $\Upsilon(s) > 0$. As the result $\mu_f(1)$ will be omitted also. The stability condition for the propagator difference scheme for ADR equation is in form:

$$\tau \leq \frac{2k}{k^2 - 2F}. \tag{64}$$

By comparing to the stability criterion (23) for the central difference scheme restriction for propagator difference scheme becomes more weak.

Secondly we consider $s_f^* \in [0, \infty)$. In case $s_f < 1$, after s is substituted by s_f^* in the right side of inequality (60) we obtain the following limiting τ:

$$\tau \leq h^2 \min\{\mu_f(0), \mu_f(s_f^*)\} =$$

$$\min\{\frac{2k}{k^2 - 2F}, \frac{1}{k + \frac{1}{4}R_e^2 v^2 (2 + kh^2) - \frac{1}{4}\sqrt{(4 + R_e^2 v^2 h^2)(R_e^2 v^2 k (4 + kh^2) + 8F)}}\} \tag{65}$$

The denominator of second term in inequality (65) should always be positive, because it is obtained from positive denominator of (60), by inserting $s = s_f^*$ and dividing with the positive expression $(2kh^2 + 8s)h^2$. It can be proved also directly. By introducing a notation $a_1 = k + \frac{1}{4}R_e^2v^2(2 + kh^2)$ and $b_1 = \frac{1}{4}\sqrt{(4 + R_e^2v^2h^2)(R_e^2v^2k(4 + kh^2) + 4k^2)}$ we can prove, that the denominator is always positive, because:

$$a_1 - b_1 = \frac{a_1^2 - b_1^2}{a_1 + b_1}. \tag{66}$$

To find a sign of the denominator (65) we need to prove that $a_1^2 - b_1^2$ is positive. In order to find it we use $F - \theta$,where θ is a small positive value and replace F by its limit value from (58). Then, because $a_1^2 - b_1^2 = \frac{1}{2}(4 + R_e^2v^2h^2) * \theta > 0$, the sign of the denominator (65) is positive.

In the case $s_f^* \geq 1$ or when $s_f \in [0, 1]$ and $s_f^* > s_f$ we obtain previous criterion (64).

If $s_f \in [0, 1]$ and $s_f^* \leq s_f$, restrictions for τ are as in expression (65).

In a special case for advection diffusion equation, when $k = 0$, $v \neq 0$, we obtain τ restriction from (65) :

$$\tau \leq \frac{2}{R_e^2v^2 - \sqrt{2F(4 + R_e^2v^2h^2)}}. \tag{67}$$

The conditions (64), (65) and (67) are stability conditions for semi-implicit propagator difference scheme. By inspecting all possible cases and comparing to stability conditions for semi-implicit central difference scheme (23), (24), and (25) it is obvious that propagator difference scheme, depending from the coefficients, can be absolutely stable when fulfills (58) or gives less restriction for the time step.

Here we should mention that numerical calculations carried out by the difference scheme (42)-(43) are in very well agreement with the proposed criterions (64), (65) and (67), including the absolutely stability feature, when criterion (58) is fulfilled. However, depended on a strategy of time step choice, relatively smooth transition from stability to instability of the semi-implicit propagator difference scheme is observed in the vicinity of time step τ criterions (64), (65) and (67). The time step from (64), (65) and (67) was used as estimation in a program for solving the ADR equation with the proposed semi-implicit propagator difference scheme (42)-(43).

Test examples for values of coefficients $R_e = 1$, $v = 1$ and $k = 1$ were calculated, to compare (46) Domenico analytical c_d and the propagator difference scheme solutions, and to confirm a precision order p of the difference scheme (42)-(43).

Results of the test example are in the Table 1, where N is the number of grid points, e_N is the maximal absolute error $e_N = \max_{l,i} e_N(l, i)$, where $e_N(l, i) = |c_d(t_l, x_i) - C_i^l|$, and $r_N = e_N / \max_{t_l,x_i}(c_d)$ is the maximal relative error of solutions. The maximal absolute and relative errors for steady-state solutions are denoted as e_N^s, r_N^s, and in the last two columns order of difference scheme (42)-(43) precision $p = ln\left(\frac{e_N}{e_{2N}}\right)/ln2$ for non-stedy, and $p^s = ln\left(\frac{e_N^s}{e_{2N}^s}\right)/ln2$ for steady-state solutions is given. As it is shown in the table precision of the propagator difference scheme is close to expected second order. To keep the order of precision for large grids second order precision in time for difference scheme is necessary.

Table 1. Maximum errors and numerical orders for the difference scheme (42)-(43)

N	e_N	r_N	e_N^s	r_N^s	p	p^s
21	$1.860 \cdot 10^{-5}$	$2.635 \cdot 10^{-4}$	$2.684 \cdot 10^{-6}$	$1.510 \cdot 10^{-5}$		
41	$4.704 \cdot 10^{-6}$	$6.710 \cdot 10^{-5}$	$6.739 \cdot 10^{-7}$	$3.792 \cdot 10^{-6}$	1.983343	1.993778
81	$1.234 \cdot 10^{-6}$	$1.784 \cdot 10^{-5}$	$1.714 \cdot 10^{-7}$	$9.644 \cdot 10^{-7}$	1.930546	1.975160
161	$3.663 \cdot 10^{-7}$	$5.532 \cdot 10^{-6}$	$4.571 \cdot 10^{-8}$	$2.571 \cdot 10^{-7}$	1.752245	1.906785

Acknowledgments

The authors would like to thank Prof. Harijs Kalis for their valuable comments and discussions. D.Ž. gratefully acknowledge the support of the ESF, project 2004/0001/VCD1/ESF/PIAA/04/NP/3.2.3.1/0001/0001/0063.

References

[1] C. M. Bethke. Geochemical Reaction Modeling: Concepts and Applications, Oxford University Press, New York, 1996.

[2] P. A. Domenico, An Analytical Model for Multidimensional Transport of a Decaying Contaminent Species, Journal of Hydrology, 91(1987), 49-58.

[3] P. A. Domenico and F. W. Schwarz, Physical and Chemical Hydrogeology, Wiley, New York, 1990.

[4] C. A. J. Fletcher, Computational Techniques for Fluid Dynamics 1. Springer Series in Computational Physics, Springer Verlag, 2st. edition, New York, 1991.

[5] G. E. Hammond, Difference Methods for Initial Value Problems, Interscience Publishers, New York , 1998.

[6] H. Kalis, Efficient Finite-Difference Scheme for Solving some Heat Transfer Problems with Convection in Multilayer Media, Int. journ. of Heat and Mass Transfer, 43(2000), 4467-4474.

[7] N. V. Karetkina, An Unconditionally Stable Difference Scheme for Parabolic Equations with First Derivatives, Computational Math. and Math. Physics, (1980), 20, 236-240.

[8] A. A. Samarskii and P. N. Vabishchevich, Numerical Methods of Convection-Diffusion Problem Solution, URSS, Moscow, 1998 (in russian).

[9] A.A.Samarskii,The theory of difference schemes, New York, Marcel Dekker, 2001.

[10] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions: with Formulas, Graphs, and Mathematical Tables, New York, Dover, 1974.

J.Rimšāns, D. Žaime. Propagator Method for Numerical Solution of the Cauchy Problem for ADR Equation.

Anotācija. Piedāvāta propogatora metode advekcijas-difūzijas reakcijas vienādojuma skaitliskai risināšanai, noteikti un salīdzināti stabilitātes nosacījumi pusaizklātai propagatora un centrālajai diferenču shēmām. Tiek pierādītas jaunās propagatora metodes priekšrocības- metode ir vai nu absolūti stabila vai arī uzrāda mazākus ierobežojumus laika soļa izvēlē salīdzinājumā ar pusaizklāto centrālo diferenču shēmu. Ir pierādīta propagatora shēmas absolūtā monotonitāte, kā arī pirmās kārtas telpā un otrās kārtas laikā aproksimācija.

Institute of Mathematics
and Computer Science,
University of Latvia
Riga, Rainis blvd 29

Received 29.12.2007