Adequate Numerical Solution of Air Pollution Problems by positive Difference Schemes on unbounded Domains

Dang Quang A [a,1] and Matthias Ehrhardt [b,*,2]

[a] *Institute of Information Technology, Vietnamese Academy of Science and Technology (VAST), 18 Hoang Quoc Viet Road, Cau Giay, Hanoi, Vietnam*

[b] *Institut für Mathematik, Technische Universität Berlin, Straße des 17. Juni 136, D–10623 Berlin, Germany*

Abstract

In this work we deal with the numerical solution of some problems of air pollution. Since the problems are posed on unbounded domains we have to introduce artificial boundaries to confine the computational region. We construct and analyse (discrete) *transparent boundary conditions* for an implicit difference scheme. We discuss the concepts of positivity and monotonicity of difference schemes and briefly consider these properties of difference schemes for advection–diffusion equations arising in problems of air (and water) pollution. The efficiency and accuracy of our method is illustrated by an example.

Key words: air pollution, advection–diffusion equation, monotone difference scheme, positive difference scheme, discrete transparent boundary condition

* Corresponding author.
Email addresses: `dangqa@ioit.ncst.ac.vn` (Dang Quang A), `ehrhardt@math.tu-berlin.de` (Matthias Ehrhardt).
URL: `http://www.math.tu-berlin.de/~ehrhardt/` (Matthias Ehrhardt).

[1] Supported by the Internationales Büro of the BMBF and the Vietnamese Academy of Science and Technology (VAST).
[2] Supported by the DFG Research Center MATHEON "Mathematics for key technologies" in Berlin.

1 Introduction

The process of pollutant transport and diffusion in the atmosphere (and in water) is described by the following *advection–diffusion equation* [1], [2]:

$$\frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} + v\frac{\partial \varphi}{\partial y} + (w - w_g)\frac{\partial \varphi}{\partial z} - \mu(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2}) - \frac{\partial}{\partial z}(\nu\frac{\partial \varphi}{\partial z}) + \sigma\varphi = f, \quad (1)$$

where φ is the *concentration of pollutants*, (u, v, w) are the components of the wind velocity, $w_g = \text{const.} > 0$ the falling velocity of the pollutants by gravity, f the power of the source, $\sigma = \text{const.} \geq 0$ the transformation coefficient of pollutants and μ, ν are the horizontal and vertical diffusion coefficients.

Many practical problems, for example, the substance (e.g. saline and alum) propagation in rivers [3], [4], the stationary problem of air pollution generated by a point source [5], [6] can be reduced to the *one–dimensional advection–diffusion equation*

$$\frac{\partial \varphi}{\partial t} + u\frac{\partial \varphi}{\partial x} - \mu\frac{\partial^2 \varphi}{\partial x^2} + \sigma\varphi = f, \quad x > 0, \quad t > 0. \quad (2)$$

Besides, the two–dimensional or three–dimensional equations by the *splitting method* [2] or *local one–dimensional* (LOD) method [7], [8] are also reduced to the one–dimensional equation (2) [6]. Therefore, the equation (2) has attracted great attention from many researchers. A number of numerical methods have been proposed for solving the equation (2) with various boundary conditions. One of the most popular methods used is the difference method. It is possible to use the method directly to the equation (2) or to each component equation separately after splitting by physical processes: first solve the diffusion equation by the difference method, and then solve the advection equation by the characteristic or the difference method (see [3], [4]). It should be remarked that usually mechanicians discretize the differential equation and after that solve the obtained difference equations without drawing attention to various properties of difference schemes such as approximation, stability and convergence. Therefore, the situation occurs when the computed concentration assumes *negative values*, that looses the physical meaning of a concentration. It should be emphasized that all trouble in the computational process is due to the advection term. This term destroys the self–adjoint property in space of the equation (2) and when approximating it by a difference quotient a numerical diffusion term arises. Consequently, The quality of the difference scheme is seriously affected by this artificial diffusion coefficient. If it is greater than the actual diffusion coefficient then the result of the computation is distored and doesn't agree with the physical picture of the problem. Hence, the construction of difference schemes that completely overcome or maximally decreases this phenomenon, have high order of accuracy and are easy realized is an actual requirement for engineers in the fields of environmental sciences.

In a recent work [9] Wang and Lacroix made an analysis of the phenomenon of numerical dispersion and proposed a weighted upwind difference scheme to overcome this phenomenon. Motivated by this work, we are involved in this paper from the mathematical point of view with qualitative characteristics of difference schemes and investigation of positivity of some difference schemes for advection–diffusion equations.

Our attention here is drawn to a simplified version of (1) under the following assumptions:

- The source of emission is *uniform* with the constant power Q and concentrated in the point $(0, 0, H)$, where H is the height of the smoke stack.
- The process of pollutant dispersion is a *stationary process*, the wind direction coincides with the positive direction of the x-axis and $u = u(z) > u_0 > 0$ with $u_0 = \text{const.}$.
- For the horizontal diffusion coefficient we assume $\mu = k_0 u$, $k_0 = \text{const.} > 0$.

The problem of determining the *concentration of pollutants* in this case is reduced to the following *stationary problem* (see [5], [6]):

$$u\frac{\partial\varphi}{\partial x} - w_g\frac{\partial\varphi}{\partial z} - \frac{\partial}{\partial z}\Big(\nu(z)\frac{\partial\varphi}{\partial z}\Big) + \sigma\varphi = 0, \quad x > 0, \quad z > 0, \tag{3a}$$

$$u\varphi(0, z) = Q\delta(z - H), \quad z > 0, \tag{3b}$$

$$\frac{\partial\varphi}{\partial z}(x, 0) = \alpha\varphi(x, 0), \quad x > 0, \tag{3c}$$

$$\lim_{z\to\infty}\varphi(x, z) = 0, \quad x > 0, \tag{3d}$$

where $\delta(z)$ denotes the Dirac delta function and $\alpha = \text{const.} \geq 0$ is a coefficient characterizing the reflection and adsorption of the bedding surface. For $\nu(z) = \text{const.}$ (3a) has the form of (2) where x plays the role of t and the role of x is replaced by z. Thus in the sequel both equations will be considered in parallel.

We remark that *analytic solutions* to the problem (3) can be found in some special cases (e.g. $u = \text{const.}$ in [10] and $\alpha = 0$ in [1]).

Usually, numerical methods are constructed for multi–dimensional problems by reducing them to a sequence of one–dimensional problems [7], [8]. Moreover, these schemes must preserve important features of the continuous model, such as the positivity of the solution (*monotone schemes*). These specially designed difference schemes must be accompanied with *artificial boundary conditions* to limit the computational domain appropriately. If the solution on the bounded computational domain coincides with the solution on the unbounded half–space (restricted to the bounded domain) one refers to these conditions as *transparent boundary conditions (TBC)*. Finally, these boundary conditions are designed on a discrete level directly for the chosen numerical schemes in order to conserve the monotonicity property and to prevent any unphysical reflections at these boundaries.

The paper is organized as follows. We derive in §2 the TBC for the time–dependent problem (2) and prove the well–posedness of the resulting initial boundary value problem. Afterwards we state the TBC for the stationary equation (3a) for a constant or linear coefficient $\nu(z)$ for $z > Z$. In §3 an adequate difference scheme for the stationary problem (3) is constructed. We discuss in §4 several concepts and definitions of positivity preserving schemes for stationary equations and extend afterwards the notion to time–dependent problems. In §5 we present three positive difference schemes for the transient advection–diffusion equation (2), namely the Samarskii scheme [7], the Crank–Nicolson scheme and the scheme of Wang and Lacroix [9]. Furthermore we address in §6 the question how to adequately discretize the obtained analytic TBC for a chosen full discretization proposed in §5. Instead of discretizing the analytic TBC with its singularity our strategy is to derive the *discrete TBC* of the fully discretized problem. We present two discretized TBC from the literature and give a concise derivation of the discrete TBC in case of the Crank–Nicolson scheme. Finally, we conclude in §7 with a numerical example illustrating the superiority of our approach.

2 The Transparent Boundary Conditions

We consider the pure *initial value problem* (IVP) (2)

$$\begin{aligned} \frac{\partial \varphi}{\partial t} &= \mu \frac{\partial^2 \varphi}{\partial x^2} - u \frac{\partial \varphi}{\partial x} - \sigma \varphi + f, \quad x \in \mathbb{R}, \quad t > 0, \\ \varphi(x,0) &= \varphi^I(x), \end{aligned} \tag{4}$$

which will be supplied later with appropriate boundary conditions (BCs). We shall assume that the coefficients remain constant outside of the computational domain $(0, X)$.

2.1 Derivation of the Transparent Boundary Condition

Here we determine the TBC at $x = X$, such that the solution of the resulting initial boundary value problem (IBVP) is as close as possible to the solution of the half–space problem (4) restricted to $(0, X)$. We have to assume that the initial data $\varphi^I(x) = Q\delta(x - H)$ is compactly supported in the computational domain $(0, X)$. We consider the *interior problem* (firstly with $f = 0$):

$$\begin{aligned} \varphi_t &= \mu \varphi_{xx} - u \varphi_x - \sigma \varphi + f, \qquad 0 < x < X, \quad t > 0, \\ \varphi(x, 0) &= \varphi^I(x), \qquad 0 < x < X, \\ \frac{\partial \varphi}{\partial x}(0, t) &= \alpha \varphi(0, t), \qquad t > 0, \\ \varphi_x(X, t) &= (T_X \varphi)(X, t), \qquad t > 0, \end{aligned} \tag{5}$$

and obtain the *Dirichlet–to–Neumann map* T_X by solving the *exterior problem*:

$$\begin{aligned} \gamma_t &= \mu\, \gamma_{xx} - u\, \gamma_x - \sigma\, \gamma, \qquad x > X, \quad t > 0, \\ \gamma(x, 0) &= 0, \qquad x > X, \\ \gamma(X, t) &= \Phi(t), \qquad t > 0, \qquad \Phi(0) = 0, \\ \gamma(\infty, t) &= 0, \qquad t > 0, \end{aligned} \tag{6}$$

and setting $(T_X \Phi)(t) = \gamma_x(X, t)$, $t > 0$. The problem (6) is coupled with (4) by the assumption that φ, φ_x are continuous across the artificial boundary at $x = X$. Since the initial data vanishes for $x > X$, we can solve (6) explicitly by the *Laplace–method*, i.e. we use the Laplace transformation of γ

$$\hat{\gamma}(x, s) = \int_0^\infty \gamma(x, t)\, e^{-st}\, dt,$$

where we set $s = \zeta + i\xi$, $\xi \in \mathbb{R}$, and $\zeta > 0$ is fixed, with the idea to later perform the limit $\zeta \to 0$. Now the exterior problem (6) is transformed to

$$\begin{aligned} &\mu\, \hat{\gamma}_{xx} - u\, \hat{\gamma}_x - (\sigma + s)\, \hat{\gamma} = 0, \qquad x > X, \\ &\hat{\gamma}(X, s) = \hat{\Phi}(s). \end{aligned} \tag{7}$$

The solution which decays as $x \to \infty$ is simply $\hat{\gamma}(x, s) = \hat{\Phi}(s)\, e^{\lambda(s)(x - X)}$, $x > X$, with

$$\lambda(s) = \frac{u}{2\mu} - \frac{1}{\sqrt{\mu}} \sqrt[+]{\eta + s}, \tag{8}$$

and the parameter

$$\eta = \frac{u^2}{4\mu} + \sigma \geq 0. \tag{9}$$

Consequently, the *transformed TBC* reads:

$$\hat{\varphi}_x(X, s) = \lambda(s)\, \hat{\varphi}(X, s). \tag{10}$$

Note that in (8) $\sqrt[+]{}$ denotes the branch of the square root with nonnegative real part. After an inverse Laplace transformation the *TBC* at $x = X$ reads:

$$\varphi_x(X, t) = \frac{u}{2\mu}\, \varphi(X, t) - \frac{e^{-\eta t}}{\sqrt{\mu \pi}} \frac{d}{dt} \int_0^t \frac{\varphi(X, t')\, e^{\eta t'}}{\sqrt{t - t'}}\, dt'. \tag{11}$$

We observe that (11) is non–local in t (of memory type), i.e. the computation of the solution at some time uses the solution at all previous times.

2.2 The Inhomogeneous Equation

Now we consider (4) with an *inhomogeneity* $f(x,t)$ provided that $f(x,t) = f$ is constant for $x > X$. In this case the transformed *exterior problem* is an inhomogeneous ordinary differential equation in x:

$$\begin{aligned} &\mu\,\hat\gamma_{xx} - u\,\hat\gamma_x - (\sigma+s)\hat\gamma = -s^{-1}f, \qquad x > X,\\ &\hat\gamma(X,s) = \hat\Phi(s). \end{aligned} \tag{12}$$

A (constant in x) *particular solution* reads

$$\hat\gamma^{part}(x,s) = \frac{f}{s(\sigma+s)}, \qquad x > X,$$

i.e. the general solution to (12) is

$$\hat\gamma(x,s) = \Bigl(\hat\Phi(s) - \frac{f}{s(\sigma+s)}\Bigr)\, e^{\lambda(s)(x-X)} + \frac{f}{s(\sigma+s)}, \qquad x > X,$$

with $\lambda(s)$ given in (8). Therefore the *transformed TBC* is given by:

$$\hat\gamma_x(X,s) = \lambda(s)\,\hat\Phi(s) - \lambda(s)\,\frac{f}{\sigma}\Bigl(\frac{1}{s} - \frac{1}{\sigma+s}\Bigr), \tag{13}$$

and after an inverse Laplace transformation of (13) the *TBC* reads:

$$\varphi_x(X,t) = \frac{u}{2\mu}\Bigl(\varphi(X,t) - \psi(t)\Bigr) - \frac{e^{-\eta t}}{\sqrt{\mu\pi}}\,\frac{d}{dt}\int_0^t \frac{\bigl(\varphi(X,t) - \psi(t)\bigr)\,e^{\eta t'}}{\sqrt{t-t'}}\,dt', \tag{14}$$

where $\psi(t)$ is obtained as $\psi(t) = f\mathcal{L}\{\frac{1}{s} - \frac{1}{c+s}\}^{-1}/\sigma = f(1-e^{-\sigma t})/\sigma$.

2.3 Well–posedness of the Initial Boundary Value Problem

It is well–known that the pure IVP (4) is well–posed:

Theorem 1 (Theorem 6.2.1, [11]) *The initial value problem for the equation* (4) *(with $f = 0$) is well–posed, i.e. for any time $T \geq 0$ there is a constant C_T such that any solution $\varphi(x,t)$ satisfies*

$$\|\varphi(.,t)\|_{L^2(\mathbb{R})} + \int_0^t \|\varphi_x(.,t')\|_{L^2(\mathbb{R})}\,dt' \leq C_T\,\|\varphi^I\|_{L^2(\mathbb{R})}$$

for $0 \leq t \leq T$.

However, the well–posedness of the associated IBVP (5) is not clear a-priori. While the existence of a solution to the 1D parabolic equation (5) with the

BC at $x = 0$ and the TBC (11) at $x = X$ is clear from the used construction it remains to prove the uniqueness of the solution. A straight forward calculation using the energy method, i.e. multiplying (4) with $\varphi(x,t)$ and integrating by parts in x, yields

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\,\|\varphi(.,t)\|^2_{L^2(0,X)} &= -\mu\|\varphi(.,t)\|^2_{L^2(0,X)} - u\int_0^X \varphi(x,t)\varphi_x(x,t)\,dx \\ &\quad - \sigma\|\varphi(.,t)\|^2_{L^2(0,X)} + \mu\,\varphi(x,t)\varphi_x(x,t)\big|_{x=0}^{x=X} \\ &\le \mu\,\varphi(x,t)\varphi_x(x,t)\big|_{x=0}^{x=X} \\ &= \mu\varphi(X,t)\varphi_x(X,t) - \mu\alpha\varphi^2(0,t),\end{aligned}$$

if $\sigma \ge u^2/(4\mu)$ (which can always be achieved by a change of variables). Finally, we integrate in time using *Plancherel's Theorem* for the Laplace transformation:

Theorem 2 (Plancherel's Theorem [12]) *If the function $g : \mathbb{R}^+ \to \mathbb{C}$ is continuous and satisfies an estimate*

$$|g(t)|^2 \le C\,e^{ct}, \qquad t \ge 0,$$

for some real constants C, c, then the Laplace transformation of g is an analytic function for $\mathrm{Re}\ s > c$ *and*

$$\int_0^\infty e^{-2\eta t}\,|g(t)|^2\,dt = \frac{1}{2\pi}\int_{-\infty}^\infty |\hat{g}(\eta + i\xi)|^2\,d\xi, \qquad \eta > c.$$

holds.

Extending $\varphi(X,t)$ by 0 for $t > T$ gives

$$\begin{aligned}\|\varphi(.,t)\|_{L^2(0,X)} &\le \|\varphi^I\|_{L^2(0,X)} + 2\mu\int_0^T \Big[\varphi(X,t)\varphi_x(X,t) - \alpha\varphi^2(0,t)\Big]\,dt \\ &= \|\varphi^I\|_{L^2(0,X)} + 2\mu\int_{\mathbb{R}} \lambda(i\xi)\,|\hat{\varphi}(X,i\xi)|^2\,d\xi - 2\mu\alpha\|\varphi(0,.)\|^2_{L^2(0,T)} \\ &\le \|\varphi^I\|_{L^2(0,X)} + 4\mu\int_0^\infty \mathrm{Re}\ \lambda(i\xi)\,|\hat{\varphi}(X,i\xi)|^2\,d\xi,\end{aligned}$$

since $\hat{\varphi}(X,-i\xi) = \bar{\hat{\varphi}}(X,i\xi)$, $\lambda(X,-i\xi) = \bar{\lambda}(X,i\xi)$. Now it can easily be checked that the *condition for well–posedness*

$$\mathrm{Re}\ \lambda(i\xi) \le 0, \quad \text{for} \quad \xi \in \mathbb{R},$$

with λ given by (8), is fulfilled and we can state the following main theorem.

Theorem 3 *The resulting parabolic IBVP* (5) *with the BC at $x = 0$ and the TBC* (11) *at $x = X$ is well–posed, i.e.*

$$\|\varphi(.,t)\|_{L^2(0,X)} \le \|\varphi^I\|_{L^2(0,X)}, \qquad t > 0, \tag{15}$$

and this implies uniqueness of the solution to the parabolic IBVP (5).

2.4 The Transparent Boundary condition for the stationary problem

Here we consider the stationary problem (3) and assume $\nu(z) = cz^a + b$, where a, b, $c \geq 0$ for $z > Z$. Then the Laplace transformed exterior problem for $\hat{\varphi} = \hat{\varphi}(s, z)$ reads

$$us\hat{\varphi} - w_g \frac{\partial}{\partial z}\hat{\varphi} - \frac{\partial}{\partial z}\Big(\nu(z)\frac{\partial}{\partial z}\hat{\varphi}\Big) + \sigma\hat{\varphi} = 0, \qquad z > Z, \tag{16}$$

with the condition $\hat{\varphi}(s, Z) = \Phi(s)$. We will formulate the TBC for the two most relevant cases $a = 0$ and $a = 1$.

For $a = 0$ we have the same structure as (11) and obtain

$$\varphi_z(x, Z) = -\frac{w_g}{2}\,\varphi(x, Z) - \sqrt{\frac{u}{\pi}}\, e^{-\eta x} \frac{d}{dx} \int_0^x \frac{\varphi(x', Z)\, e^{\eta x'}}{\sqrt{x - x'}}\, dx', \tag{17}$$

with the parameter $\eta = w_g^2/(4u) + \sigma \geq 0$. Here, the TBC (17) is non–local in the spatial coordinate x.

In the case of a *linear varying coefficient* $\nu(z)$, i.e. $a = 1$, the explicit solution to (16) decaying for $z \to \infty$ is the following ratio of two Hankel functions of the second kind

$$\hat{\varphi}(s, z) = \Phi(s) \left(\frac{cz + b}{cZ + b}\right)^{-\frac{w_g}{2c}} \frac{H^{(2)}_{-\frac{w_g}{c}}\left(2\sqrt{-su - \sigma}\sqrt{\frac{cz+b}{c^2}}\right)}{H^{(2)}_{-\frac{w_g}{c}}\left(2\sqrt{-su - \sigma}\sqrt{\frac{cZ+b}{c^2}}\right)}, \quad z > Z. \tag{18}$$

The Hankel functions of the second kind (and order n) are defined as $H_n^{(2)}(\zeta) := J_n(\zeta) - iY_n(\zeta)$ where $J_n(\zeta)$ is a Bessel function of the first kind and $Y_n(\zeta)$ is a Bessel function of the second kind. The expression (18) can be inverse transformed (numerically) to obtain a TBC.

We remark that in the classical model of Judin and Schwez from 1940 [1] it is assumed that $a = 1$ holds in the domain $z < Z$ and $a = 0$ for $z > Z$. For a detailed discussion of different models of the vertical diffusion coefficient $\nu(z)$ we refer the reader to [1, Chapter 1.5].

3 The Finite Difference Scheme

In this section we construct a difference scheme for the stationary problem (3). Let us introduce the grid points $x_n = n\Delta x$, $z_j = j\Delta z$, $n, j = 0, 1, \ldots,$ where

$\tau = \Delta x$, $h = \Delta z$ denote the step sizes in x and z direction. Furthermore we assume that $H = z_{j_H}$, i.e. the source is located at the grid point $z = z_{j_H}$.

In the sequel we want to construct a *monotone finite difference scheme* (cf. Definition 5) and follow closely the ideas of Samarskii [7]. To do so, we rewrite (3a) in the form

$$u\frac{\partial \varphi}{\partial x} = L\varphi, \qquad x > 0, \quad z > 0,$$

with

$$L\varphi = \frac{\partial}{\partial z}\Big(\nu\frac{\partial \varphi}{\partial z}\Big) + w_g\frac{\partial \varphi}{\partial z} - \sigma\varphi.$$

To obtain a *monotone scheme*, we introduce the *perturbed operator* $\tilde{L}$

$$\tilde{L}\varphi = \chi(z)\frac{\partial}{\partial z}\Big(\nu(z)\frac{\partial \varphi}{\partial z}\Big) + w_g\frac{\partial \varphi}{\partial z} - \sigma\varphi, \tag{19}$$

where

$$\chi(z) = \frac{1}{1+R(z)}, \quad R(z) = \frac{w_g\Delta z}{2\nu(z)}.$$

The coefficient $R(z)$ is called the *Reynolds difference number*.

Now the operator $\tilde{L}$ is approximated by the *difference operator*

$$\tilde{L}_h\varphi_j^n = \chi_j D_h^+\Big(a_j D_h^-\varphi_j^n\Big) + b_j a_{j+1} D_h^+\varphi_j^n - \sigma\varphi_j^n, \tag{20}$$

with $\chi_j = 1/(1+R(z_j))$, $a_j = \nu_{j-1/2} = \nu(z_j - h/2)$ and $b_j = w_g/\nu_j$, $\nu_j = \nu(z_j)$. Here, D_h^+, D_h^- denote the usual forward and backward difference quotients.

The initial condition (3b) is approximated through the discrete delta function

$$\varphi_j^0 = \begin{cases} \frac{Q}{hu_{j_H}}, & j = j_H, \\ 0, & \text{else.} \end{cases} \tag{21}$$

In order to approximate the boundary condition (3c) at the ground $z = 0$ we choose the centered difference quotient

$$\frac{\varphi_1^n - \varphi_{-1}^n}{2h} = \alpha\varphi_0^n, \quad n \geq 0, \tag{22}$$

with the fictitious grid point $z_{-1} = -h$. The proper incorporation of the decay condition (3d) into the finite difference scheme by introducing a so–called *discrete transparent boundary condition* will be outlined in §6.

We shall consider the *implicit finite difference method*

$$u_j D_\tau^+\varphi_j^n = \tilde{L}_h\varphi_j^{n+1}, \tag{23}$$

which has the discretization error $\mathrm{O}(h^2+\tau)$ [7]. The numerical scheme (23) reads

$$u_j \frac{\varphi_j^{n+1}-\varphi_j^n}{\tau} = \frac{\chi_j}{h}\Big(a_{j+1}\frac{\varphi_{j+1}^{n+1}-\varphi_j^{n+1}}{h} - a_j\frac{\varphi_j^{n+1}-\varphi_{j-1}^{n+1}}{h}\Big)$$
$$+ b_j a_{j+1}\frac{\varphi_{j+1}^{n+1}-\varphi_j^{n+1}}{h} - \sigma\varphi_j^{n+1}, \quad j,n=0,1,\dots.$$

This second order difference equation can be written in the standard form [7]:

$$A_j\varphi_{j-1}^{n+1} - C_j\varphi_j^{n+1} + B_j\varphi_{j+1}^{n+1} = -F_j^n, \quad j,n=0,1,2,\dots, \tag{24}$$

where we assumed that φ_j^n is known. The coefficients in (24) are given by

$$\begin{aligned} A_j &= \rho\chi_j a_j, \\ B_j &= \rho\chi_j a_{j+1} + \rho h b_j a_{j+1}, \\ C_j &= A_j + B_j + u_j + \sigma\tau, \\ F_j^n &= u_j\varphi_j^n, \end{aligned}$$

with the parabolic mesh ratio $\rho = \tau/h^2$. Setting $j=0$ in (24) we obtain from (22) the *boundary condition*

$$\varphi_0^{n+1} = \alpha_1\varphi_1^{n+1} + \beta_1,$$

where

$$\alpha_1 = \frac{A_0+B_0}{C_0+2h\alpha A_0}, \quad \beta_1 = \frac{F_0}{C_0+2h\alpha A_0}.$$

Alternatively, one can consider the *Crank–Nicolson discretization*

$$u_j D_\tau^+\varphi_j^n = \tilde{L}_h\frac{\varphi_j^{n+1}+\varphi_j^n}{2}, \quad n\ge 0, \tag{25}$$

with the discretization error $\mathrm{O}(h^2+\tau^2)$.

4 About the Positivity and the Monotonicity of Difference Schemes

The main concepts of the theory of difference scheme are systematically presented in the books, e.g. [7], [13]. They are approximation, stability and convergence. The stability is the inside property of difference scheme. It guarantees that the computational error does not accumulate in the process of computation from time to time. Meanwhile the concepts of approximation and convergence associate difference scheme with the discretized differential problem. Besides the above properties which are necessarily drawn attention in constructing difference schemes, for many problems of hydrodynamics, mass and heat transfer,... one is interested in the more thin properties. It is positivity and monotonicity properties.

Definition 4 (positive scheme [14]) *A difference scheme is called* positive *if its solution is non–negative when its right hand side, initial condition and boundary conditions are all non–negative.*

Definition 5 (monotone scheme [14]) *A difference scheme is called* monotone *if it preserves the monotonicity in the same direction of space profiles when passing from one time step to another.*

The concepts of positive and monotone difference scheme have clear physical meanings. But to discover whether a difference scheme has these properties, especially the property of monotonicity, is not easy.

For hyperbolic equations with constant coefficients Friedrichs [15] introduced the following concept of difference schemes with positive approximation. Consider an equation with one space variable. In the domain of definition of the problem let us introduce a grid with space step h and the time step τ. Denote the grid function by y with value $y_j^n = y(jh, n\tau)$.

Definition 6 (positive approximation [15]) *A difference scheme for an evolution equation with constant coefficients has a* positive approximation *if for zero right hand side it has the form*

$$y_j^{n+1} = \sum_{\mu,\nu} \alpha_\mu^\nu y_{j+\mu}^{n+\nu}, \tag{26}$$

where $\alpha_\mu^\nu \geq 0$, for all ν, μ are positive coefficients.

The following proposition is easy to verify by definition.

Proposition 7 *Let* (26) *be an explicit difference scheme, i.e., $\nu \leq 0$. If it has a positive approximation then it is positive and monotone.*

PROOF. Since (26) has a positive approximation we have by definition $\alpha_\mu^\nu \geq 0$ for all ν and μ. Therefore, $y_j^{n+1} \geq 0$ if boundary and initial conditions are all non–negative. It means that the difference scheme is positive in the sense of Definition 4.

Now, let all layers $y^{n+\nu}$ be monotone grid functions of the same direction, say, nondecreasing functions. It means that $\forall j, \mu\, y_{j+\mu}^{n+\nu} \leq y_{j+1+\mu}^{n+\nu}$. Therefore,

$$y_j^{n+1} - y_{j+1}^{n+1} = \sum_{\mu,\nu} \alpha_\mu^\nu (y_{j+\mu}^{n+\nu} - y_{j+1+\mu}^{n+\nu}) \leq 0.$$

So, y^{n+1} is a nondecreasing grid function. Thus, the difference scheme is monotone in the sense of Definition 5.

Samarskii [7] introduced another definition of monotone difference schemes, which in essence is a criteria for positive difference schemes in the sense of Definition 4. This concept is introduced first for stationary equations and afterwards extended for evolution equations.

Definition 8 (monotone scheme [7]) *The difference scheme* $L_h y_j = f_j$ *is called* monotone *if it has the form*

$$L_h y_j = -A_j y_{j-1} + C_j y_j - B_j y_{j+1} = f_j, \qquad j = 1, \ldots, N-1, \tag{27a}$$

where

$$A_j > 0,\ B_j > 0,\ C_j > 0 \text{ and } C_j - A_j - B_j \geq 0. \tag{27b}$$

The operator L_h herein is called *monotone operator*.

The monotone (in the above sense) difference scheme satisfies a *discrete maximum principle*, namely, if $L_h y_j \geq 0$ for any j and the grid function y_j is not a constant then it can not reach a negative minimum at inner points (see [7], Chap.1). Therefore, the solution of the monotone difference scheme is non–negative if the right hand side $f_j \geq 0$ and the boundary conditions $y_0, y_N \geq 0$. The sense of monotonicity maybe comes from the fact that if $C_j = A_j + B_j$, $f_j = 0$ for all $j = 1, \ldots, N-1$ then the grid solution of (27a) is a monotone function. Moreover, in the case $f_j \geq 0$ if $y_0 \geq y_1$ it is easy to show that the grid solution y_j is a decreasing function.

In [7] there is no definition of monotone difference schemes for evolution equations. Below we state the following

Definition 9 (monotone scheme for evolution equation) *A difference scheme for an evolution equation is called* monotone *if it satisfies a discrete maximum principle, namely, if the difference scheme* $L_h(y_j^n, y_j^{n+1}) = f_j^n$ *with given initial and boundary conditions satisfies the condition* $L_h(y_j^n, y_j^{n+1}) \geq 0$ *then its solution cannot reach a negative minimum at inner points.*

Proposition 10 *The purely implicit difference scheme*

$$\frac{y_j^{n+1} - y_j^n}{\tau} + L_h y_j^{n+1} = f_j^n, \tag{28}$$

where L_h *is a monotone operator, is monotone in the sense of Definition 9 and is positive in the sense of Definition 4.*

PROOF. Let L_h be a monotone operator. Then it has the form

$$L_h y_j^{n+1} = -A_j^{n+1} y_{j-1}^{n+1} + C_j^{n+1} y_j^{n+1} - B_j^{n+1} y_{j+1}^{n+1}, \qquad j = 1, \dots, N-1, \quad \text{(29a)}$$

where

$$A_j^{n+1} > 0,\ B_j^{n+1} > 0,\ C_j^{n+1} > 0 \text{ and } C_j^{n+1} - A_j^{n+1} - B_j^{n+1} \geq 0. \qquad \text{(29b)}$$

We shall prove first that the difference scheme (28) is monotone in the sense of Definition 9, i.e. if $f_j^n \geq 0$ for any j and n then the grid solution y cannot reach a negative minimum at a point with the indexes $0 < j < N$ and $n > 0$. In order to do this we assume that the grid function y reaches a negative minimum at a point $(j_0, n+1)$ with $0 < j_0 < N$ and $n \geq 0$. Then among the neighbouring points $(j_0 - 1, n+1)$, $(j_0 + 1, n+1)$ and (j_0, n) there exist at least one point, where the function y assumes a value, which is strictly greater than $y_{j_0}^{n+1}$. Now, in view of (29a) we have

$$\begin{aligned} L_h y_{j_0}^{n+1} &= -A_{j_0}^{n+1} y_{j_0-1}^{n+1} + C_{j_0}^{n+1} y_{j_0}^{n+1} - B_{j_0}^{n+1} y_{j_0+1}^{n+1} \\ &= A_{j_0}^{n+1}(y_{j_0}^{n+1} - y_{j_0-1}^{n+1}) + B_{j_0}^{n+1}(y_{j_0}^{n+1} - y_{j_0+1}^{n+1}) \\ &\quad + (C_{j_0}^{n+1} - A_{j_0}^{n+1} - B_{j_0}^{n+1}) y_{j_0}^{n+1}. \end{aligned}$$

Consequently, the equation (28) at the point $(j_0, n+1)$ becomes

$$\begin{aligned} \frac{y_{j_0}^{n+1} - y_{j_0}^n}{\tau} &+ A_{j_0}^{n+1}(y_{j_0}^{n+1} - y_{j_0-1}^{n+1}) + B_{j_0}^{n+1}(y_{j_0}^{n+1} - y_{j_0+1}^{n+1}) \\ &+ (C_{j_0}^{n+1} - A_{j_0}^{n+1} - B_{j_0}^{n+1}) y_{j_0}^{n+1} = f_j^n. \end{aligned} \qquad (30)$$

Due to the conditions (29b) and the property of the point $(j_0, n+1)$ the left hand side of (30) is strictly less than zero while the right hand side is non–negative. This contradiction proves that the grid solution y cannot reach a negative minimum at an interior point. Thus, the difference scheme (28) is monotone in the sense of Definition 9. The positivity of the difference scheme (28) is a straightforward corollary of its monotonicity and the proof of the Proposition is completed.

We remark that the notion of *monotone difference schemes* by Definition 5 is very rigorous and in the literature on difference schemes the concept of monotonicity associated with the maximum principle is commonly used (see [16] and the references therein). Using the above concepts we investigate in the next section the positivity of difference schemes for advection–diffusion equations.

5 Positive difference Schemes for Advection–Diffusion Equations

We rewrite the equation (2) with the variable diffusion coefficient $k(x,t)$ in the form

$$\frac{\partial \varphi}{\partial t} + L\varphi = f, \tag{31a}$$

where

$$L\varphi = -\frac{\partial}{\partial x}(k\frac{\partial \varphi}{\partial x}) + u\frac{\partial \varphi}{\partial x} + \sigma\varphi. \tag{31b}$$

(1) Following Samarskii [7] we construct a difference scheme for the perturbed equation associated with the equation (31a), namely, for the equation (31a) with L replaced by

$$\tilde{L}\varphi = -\chi\frac{\partial}{\partial x}(k\frac{\partial \varphi}{\partial x}) + u\frac{\partial \varphi}{\partial x} + \sigma\varphi,$$

where $\chi = 1/(1+R)$ and $R = 0.5h|u|/k$.

The difference scheme for the case of a positive velocity $u \geq 0$ has the form

$$\frac{y_j^{n+1} - y_j^n}{\tau} + \tilde{L}_h y_j^{n+1} = f_j^n, \tag{32}$$

where

$$\begin{aligned} \tilde{L}_h y_j &= -\chi D_h^+(a_j^n D_h^- y_j) + b_j^n D_h^- y_j + \sigma y_j, \\ a_j^n &= k(x_j - 0.5h, t_n - 0.5\tau), \quad b_j^n = u(x_j, t_n - 0.5\tau). \end{aligned} \tag{33}$$

D_h^+ and D_h^- are the usual forward and backward difference quotients with step size h. It is easy to prove that the difference scheme (32), (33) has the approximation error $\mathrm{O}(\tau + h^2)$ on smooth solutions of (31) and is monotone for any τ and h. More precisely, $\tilde{L}_h$ is monotone. Therefore, the solution of the difference scheme is non–negative when the right hand side, initial and boundary conditions are non–negative. The difference schemes of the type (32), (33) are used in [5], [6] for a problem of air pollution.

(2) Next we consider the *Crank–Nicolson difference scheme* associated with (32)

$$\frac{y_j^{n+1} - y_j^n}{\tau} + \tilde{L}_h \frac{y_j^{n+1} + y_j^n}{2} = f_j^{n+1/2}. \tag{34}$$

Suppose $\tilde{L}_h y_j = -A_j y_{j-1} + C_j y_j - B_j y_{j+1}$. Of course, the coefficients satisfy (27b). From (34) we have

$$\begin{aligned} &-0.5\tau A_j y_{j-1}^{n+1} + (1 + 0.5\tau C_j) y_j^{n+1} - 0.5\tau B_{j+1}^{n+1} \\ &\qquad = -0.5\tau A_j y_{j-1}^n + (1 - 0.5\tau C_j) y_j^n + 0.5\tau B_{j+1}^n + \tau f_j^{n+1/2}. \end{aligned}$$

Obviously, the operator on the left side is monotone and if $1-0.5\tau C_j \geq 0$ then (34) is a positive difference scheme. For the case k = const. this condition is satisfied if

$$\frac{\tau}{h^2} < \frac{1}{2k + h \max u}.$$

Thus, although the Crank–Nicolson scheme has the approximation error $\mathrm{O}(\tau^2 + h^2)$ due to the above limitation the second order accuracy in time has no more meaning.

(3) Finally, let us consider the difference scheme proposed by *Wang and Lacroix* [9]. This scheme has the form of (34) with

$$\begin{aligned}\tilde{L}_h y_j &= -k D_h^2 y_j + u[(0.5+\alpha) D_h^- y_j + (0.5-\alpha) D_h^+ y_j] \\ &= -k D_h^2 y_j + u D_h^0 y_j,\end{aligned} \tag{35}$$

where $\alpha \in [-0.5, 0.5]$ and $D_h^2 = D_h^+ D_h^-$, D_h^0 are the second order and the first order centered difference quotients. It is easy to show that the sufficient condition for that the difference scheme (35) has second order of approximation in h is $\alpha = \mathrm{O}(h)$ and the sufficient conditions for the difference scheme (35) to have the positivity property are

$$h \leq \frac{2k}{\max u}, \quad \frac{\tau}{h} \leq \frac{2}{\max u}, \quad \frac{\tau}{h^2} \leq \frac{1}{k + 2\alpha h \max u}.$$

Thus, theoretically the Wang–Lacroix scheme is also more complicated than the scheme (34) with $\tilde{L}_h$ defined by (33) but it is not better in the sense of approximation and positivity.

6 The Discrete Transparent Boundary Condition

Next we shall address the question how to adequately discretize the analytic TBC (11) for a chosen full discretization of (4) proposed in Section 5. Instead of discretizing the analytic TBC (11) with its singularity our strategy is to derive the *discrete TBC* of the fully discretized problem. With the uniform grid points $x_j = j\Delta x$, $t_n = n\Delta t$ ($h = \Delta x$, $\tau = \Delta t$) and the approximation $\varphi_j^n \approx \varphi(x_j, t_n)$ the Crank–Nicolson scheme (34) for solving (31b) reads (for $k(x)$ = const. and $f_j^{n+1/2} = 0$):

$$D_\tau^+ \varphi_j^n = \mu\, D_h^2 \varphi_j^{n+1/2} - u\, D_h^+ \varphi_j^{n+1/2} - \sigma\, \varphi_j^{n+1/2}, \qquad j \geq 0, \tag{36}$$

with $\mu = k/(1+R)$ the abbreviation $\varphi_j^{n+1/2} = (\varphi_j^{n+1} + \varphi_j^n)/2$. While a uniform grid in x is necessary in the exterior domain, the interior grid may be nonuniform in x.

We remind the reader that In the scheme (36) D_τ^+ denotes the usual forward and D_h^2 the second order difference quotient:

$$D_\tau^+ \phi_j^n = \frac{\varphi_j^{n+1} - \varphi_j^n}{\tau}, \qquad D_h^2 \varphi_j^{n+1/2} = \frac{\varphi_{j+1}^{n+1/2} - 2\,\varphi_j^{n+1/2} + \varphi_{j-1}^{n+1/2}}{h^2}.$$

The advection term is discretized by the backward difference quotient

$$D_h^- \varphi_j^n = \frac{\varphi_j^n - \varphi_{j-1}^n}{h},$$

('upwind differencing') since the velocity is positive: $u \geq 0$.

6.1 *Discretization strategies for the TBC*

Here we want to compare three strategies to discretize the TBC (11) which is a rather delicate question with its mildly singular convolution kernel. First we review two known discretization techniques from Mayfield [17] and Halpern [18].

Discretized TBC of Mayfield

To compare our results we first consider the *ad-hoc discretization strategy of Mayfield* for the Schrödinger equation applied to the advection–diffusion equation (4). According to the approach of Mayfield [17] one way to discretize the analytic TBC (11) at $x = X$ (with $Jh = X$) in the equivalent form

$$\varphi(X,t) = \sqrt{\frac{\mu}{\pi}} \int_0^t \frac{\varphi_x(X,t')\, e^{-\eta(t-t')}}{\sqrt{t-t'}}\, dt' - \frac{u}{2\sqrt{\mu\pi}} \int_0^t \frac{\varphi(X,t')\, e^{-\eta(t-t')}}{\sqrt{t-t'}}\, dt', \quad (37)$$

with η given by (9), is for the first integral

$$\int_0^t \frac{\varphi_x(X,t-t')\, e^{-\eta t'}}{\sqrt{t'}}\, dt' \approx \frac{1}{h} \sum_{m=0}^{n-1} (\varphi_J^{n-m} - \varphi_{J-1}^{n-m})\, e^{-\eta m\tau} \int_{t_m}^{t_{m+1}} \frac{dt'}{\sqrt{t'}}$$
$$= \frac{2\sqrt{\tau}}{h} \sum_{m=0}^{n-1} \frac{(\varphi_J^{n-m} - \varphi_{J-1}^{n-m})\, e^{-\eta m\tau}}{\sqrt{m+1} + \sqrt{m}}.$$

Discretizing the second integral in (37) analogously leads to the following *discretized TBC* for the advection–diffusion equation (4):

$$\varphi_{J-1}^n - \Bigl(1 + \frac{uh}{2\mu}\Bigr)\varphi_J^n = \frac{\sqrt{\pi}h}{2\sqrt{\mu\tau}}\varphi_J^n + \sum_{m=1}^{n-1} \tilde{\ell}^{(m)}(\varphi_J^{n-m} - \varphi_{J-1}^{n-m}) - \frac{uh}{2\mu}\sum_{m=1}^{n-1} \tilde{\ell}^{(m)}\varphi_J^{n-m}, \quad (38)$$

with the convolution coefficients $\tilde{\ell}^{(m)}$ given by

$$\tilde{\ell}^{(m)} = \frac{e^{-\eta m\tau}}{\sqrt{m+1} + \sqrt{m}},$$

and η defined by (9). On the fully discrete level (38) is not perfectly transparent any more and may possibly lead to an unstable numerical scheme as shown by Mayfield [17] in case of the Schrödinger equation.

Artificial BC of Halpern

Secondly we present the *approach of Halpern* [18] which was generalized by Lohéac in [19] to the case that the diffusion coefficient μ in (4) can depend on x. In [18] Halpern developed a family of artificial boundary conditions for the linear advection–diffusion equation with small diffusion μ. To start with we rewrite the transformed TBC (10) as

$$\hat{\varphi}_x(X,s) = \frac{1}{2\mu}\left(u - \sqrt[+]{u^2 + 4(\sigma+s)\mu}\right)\hat{\varphi}(X,s). \quad (39)$$

Now Halpern's approach consists of using Taylor or Padé approximations of the term in parentheses in (39) with respect to a small value of μ in order to obtain a local in t boundary condition. A first order Taylor approximation gives

$$u - \sqrt[+]{u^2 + 4(\sigma+s)\mu} \approx u - |u| + \frac{2\mu(\sigma+s)}{|u|},$$

which leads to the transformed artificial boundary condition

$$\hat{\varphi}_x(X,s) = \left(\frac{u-|u|}{2\mu} + \frac{\sigma+s}{|u|}\right)\hat{\varphi}(X,s). \quad (40)$$

Since $u > 0$ we have an *outflow BC at $x = X$* and an inverse Laplace transformation of (40) yields the *first order artificial boundary condition*:

$$\varphi_t(X,t) - u\,\varphi_x(X,t) + \sigma\,\varphi(X,t) = 0. \quad (41)$$

To discretize (41) at $X = Jh$ we follow the suggestion in [18] and obtain:

$$D_\tau^+ \varphi_J^n - u\, D_h^- \varphi_J^{n+1/2} + \sigma\, \varphi_J^{n+1/2} = 0. \tag{42}$$

While Halpern showed that the interior Crank–Nicolson scheme together with the artificial boundary condition (42) (for $\sigma = 0$) is stable and has order two in time and space, the resulting scheme suffers from reduced accuracy as we will see later in the numerical examples of §7.

The Discrete TBC

In order to avoid any numerical reflections at the artificial boundary and to ensure unconditional stability of the resulting scheme we will construct in the next subsection a *discrete TBC* instead of choosing an ad–hoc discretization of the analytic TBC (11) like Mayfields approach or the approach of Halpern. The discrete TBC completely avoids any numerical reflections at the boundary at no additional computational costs (compared to ad–hoc discretization strategies like (38)).

6.2 The Derivation of the Discrete TBC

We mimic the derivation from § 2 on a discrete level: we obtain the discrete TBC at $x_J = X$ by solving the *discrete exterior problem*, i.e. (36) for $j \geq J-1$:

$$\Delta_\tau^+ \varphi_j^n + u\frac{\tau}{h}\Delta_h^- \varphi_j^{n+1/2} + 2\kappa \varphi_j^{n+1/2} = r\Delta_h^2 \varphi_j^{n+1/2}, \tag{43}$$

where $r = \mu\,\tau/h^2$ denotes the *(parabolic) mesh ratio*, $\kappa = \sigma\tau/2$. In the scheme (43) we used the difference operators $\Delta_\tau^+ = \tau\, D_\tau^+$, $\Delta_h^2 = h^2\, D_h^2$, etc. To proceed, we apply the *$\mathcal{Z}$–transformation*:

$$\mathcal{Z}\{\varphi_j^n\} = \hat{\varphi}_j(z) := \sum_{n=0}^{\infty} \varphi_j^n\, z^{-n}, \qquad z \in \mathbb{C}, \quad |z| > R_{\hat{\varphi}},$$

j fixed ($R_{\hat{\varphi}}$ denotes the convergence radius of the Laurent series), to solve (43) explicitly. We assume for the initial data $\varphi_j^0 = 0,\ j \geq J-1$, and obtain the *transformed exterior scheme*

$$\frac{2}{r}\frac{z-1}{z+1}\,\hat{\varphi}_j(z) + \Big[P_e\Delta_h^- + \frac{2\kappa}{r}\Big]\hat{\varphi}_j(z) = \Delta_h^2 \hat{\varphi}_j(z), \quad j \geq J-1, \tag{44}$$

with $P_e = uh/\mu$. The two linearly independent solutions of the resulting *second order difference equation* (44) take the form

$$\hat{\varphi}_j(z) = \nu_{1,2}^{j+1}(z), \quad j \geq J-1, \tag{45}$$

where $\nu_{1,2}(z)$ are the solutions of the quadratic equation

$$\nu^2 - 2\left[1 + \frac{1}{r}\Big(\frac{z-1}{z+1} + \kappa\Big) + \frac{Pe}{2}\right]\nu + 1 + Pe = 0, \tag{46}$$

i.e. they can be written as

$$\nu_{1,2}(z) = 1 + \frac{Pe}{2} + \frac{1}{r}\Big(\frac{z-1}{z+1} + \kappa\Big) \pm \sqrt[+]{Az^2 - 2Bz + C}.$$

Since we are seeking decreasing modes as $j \to \infty$ we have to require $|\nu_2(z)| < 1$ and obtain the $\mathcal{Z}$–transformed *discrete TBC* as

$$(1 + Pe)\,\hat{\varphi}_{J-1}(z) = \nu_1(z)\,\hat{\varphi}_J(z), \tag{47}$$

where we have used the property $\nu_1(z)\nu_2(z) = 1 + Pe$. It was shown by Lill [20, Theorem 3.11] that for the solutions to the quadratic equation (46) $|\nu_1(z)| > 1$, $|\nu_2(z)| < 1$ holds for $|z| > 1$.

It only remains to inverse $\mathcal{Z}$–transform $\nu_1(z)$ in order to obtain the discrete TBC from (47) and in a tedious calculation this can be performed explicitly [21], [22]. This yields the following *discrete TBC*:

$$(1 + Pe)\,\varphi_{J-1}^n = \ell^{(n)} * \varphi_J^n = \sum_{k=1}^{n} \ell^{(n-k)}\varphi_J^k, \quad n \geq 1, \tag{48}$$

with convolution coefficients $\ell^{(n)}$ given by

$$\begin{aligned} \ell^{(0)} &= H + \frac{\kappa}{r} + \frac{1+\sqrt{A}}{r} \\ \ell^{(n)} &= \frac{2(-1)^n}{r} + \frac{1}{r\sqrt{A}}\cdot \\ &\quad \cdot \left(A\widetilde{P}_n(\upsilon) + C\widetilde{P}_{n-1}(\upsilon) + 4\sum_{k=0}^{n-1}(-1)^{n-k}\widetilde{P}_k(\upsilon)\right), \quad n \geq 1, \end{aligned} \tag{49}$$

where the constants can be determined as

$$\begin{aligned} A &= (\kappa^+)^2 + 2rH\kappa^+ + \beta^2, \\ B &= \kappa^+\kappa^- - 2rH\kappa - \beta^2, \\ C &= (\kappa^-)^2 - 2rH\kappa^- + \beta^2, \end{aligned}$$

with $H = 1 + Pe/2$, $\kappa^+ = 1 + \kappa$, $\kappa^- = 1 - \kappa$, $\beta = u\tau/(2h)$. The parameters λ, υ are given by

$$\lambda = \frac{\sqrt{A}}{\sqrt[+]{C}}, \qquad \upsilon = \frac{B}{\sqrt{A}\sqrt[+]{C}}. \tag{51}$$

$\widetilde{P}_n(\upsilon) := \lambda^{-n}P_n(\upsilon)$ denotes the *"damped" Legendre polynomials* ($\widetilde{P}_0 \equiv \lambda^{-1}$, $\widetilde{P}_{-1} \equiv 0$) and δ_n^0 is the Kronecker symbol.

Remark 11 (Implicit Euler scheme) *For the implicit Euler scheme we obtain the coefficients (cf. [22]):*

$$\begin{aligned}
\ell^{(0)} &= H + \frac{\kappa}{r} + \frac{1+\sqrt{A}}{2r}, \\
\ell^{(1)} &= -\frac{1}{2r} + \frac{1}{2r\sqrt{A}}\Big(A\widetilde{P}_1(v) - 2B\Big) = -\frac{1}{2r}\left(1+\frac{B}{\sqrt{A}}\right), \\
\ell^{(n)} &= \frac{1}{2r\sqrt{A}}\Big(A\widetilde{P}_n(v) - 2B\widetilde{P}_{n-1}(v) + C\widetilde{P}_{n-2}(v)\Big), \quad n \geq 2.
\end{aligned} \tag{52}$$

6.3 The Inhomogeneous Equation

Analogously to §2.2 we consider the discrete equation (36) with an *inhomogeneity* $f_j^{n+1/2}$ provided that $f_j^{n+1/2} = f = \text{const.}$ for $j \geq J-1$. In this case the transformed *discrete exterior problem* is an inhomogeneous ordinary difference equation in j:

$$2\frac{z-1}{z+1}\,\hat{\varphi}_j(z) + \Big[rP_e\Delta_h^- + 2\kappa\Big]\hat{\varphi}_j(z) = r\Delta_h^2\hat{\varphi}_j(z) + \tau f\frac{z}{z-1}, \quad j \geq J-1, \tag{53}$$

and a (constant in j) *particular solution* of (53) reads

$$\hat{\varphi}_j^{part}(z) = \frac{\tau f}{2}\frac{z}{z-1}\frac{z-1+\kappa(z+1)}{z+1}, \qquad j > J-1, \tag{54}$$

i.e. the general solution to (53) is

$$\hat{\varphi}_j(z) = \frac{\hat{\varphi}_J - \hat{\varphi}_j^{part}(z)}{1+P_e}\nu_1^{j-J}(z) + \hat{\varphi}_j^{part}(z), \qquad j > J-1,$$

with ν_1 solution of (46) with $|\nu_1(z)| > 1$. Thus the *transformed discrete TBC* is given by:

$$(1+P_e)\,\hat{\varphi}_{J-1}(z) = \Big(\hat{\varphi}_J - \hat{\varphi}_j^{part}(z)\Big)\nu_1(z) + (1+P_e)\,\hat{\varphi}_j^{part}(z).$$

After an inverse $\mathcal{Z}$–transformation the *discrete TBC* reads:

$$(1+P_e)\,\varphi_{J-1}^n = \sum_{k=1}^{n}\ell^{(n-k)}\varphi_J^k - \sum_{k=1}^{n}\psi^{(n-k)}\varphi_J^k + (1+P_e)\,\psi^{(n)}, \quad n \geq 1, \tag{55}$$

with $\ell^{(n)}$ given by (49) and $\psi^{(n)}$ is obtained from (54) by an inverse $\mathcal{Z}$–transformation:

$$\psi^{(n)} = \mathcal{Z}^{-1}\{\hat{\varphi}_j^{part}(z)\} = \frac{\tau f}{2}(-1)^n + \left(\frac{\tau}{2}\right)^2\sigma f. \tag{56}$$

Note that it is also possible to derive a (discrete) TBC in the case of a space–dependent inhomogeneity $f = f_j$, $j \geq J-1$, using the techniques developed in [22, Chapter 1.3]. However, the computational costs for evaluating this (discrete) TBC are unacceptable high.

6.4 The summed convolution coeffcients

In this subsection we want to investigate the asymptotic behaviour of the convolution coefficients $\ell^{(n)}$ given by (49). We will see that it is beneficial to reformulate the discrete TBC (48) and give a recursion formula for these new coefficients.

It can be shown [22] that the convolution coefficients (49) have the asymptotic behaviour $\ell^{(n)} \sim 4(-1)^n/r$, $n \to \infty$ and this alternating behaviour may lead to subtractive cancellation in (48). Therefore we prefer to use the following *summed coefficients* in the implementation

$$s^{(n)} := \ell^{(n)} + \ell^{(n-1)}, \quad n \geq 1, \quad s^{(0)} := \ell^{(0)},$$

and compute

$$\begin{aligned} s^{(n)} &= \frac{1}{r\sqrt{A}} \Big(A\widetilde{P}_n(\upsilon) + [A + C - 4]\, \widetilde{P}_{n-1}(\upsilon) + C\widetilde{P}_{n-2}(\upsilon) \Big) \\ &= \frac{1}{r\sqrt{A}} \Big(A\widetilde{P}_n(\upsilon) - 2B\widetilde{P}_{n-1}(\upsilon) + C\widetilde{P}_{n-2}(\upsilon) \Big) \\ &= \frac{\sqrt{A}}{2r} \Big(\widetilde{P}_n(\upsilon) - 2\upsilon\lambda^{-1}\widetilde{P}_{n-1}(\upsilon) + \lambda^{-2}\widetilde{P}_{n-2}(\upsilon) \Big). \end{aligned} \tag{57}$$

Using

$$\upsilon\lambda^{-1}\widetilde{P}_{n-1}(\upsilon) = \frac{n}{2n-1}\widetilde{P}_n(\upsilon) + \frac{n-1}{2n-1}\lambda^{-2}\widetilde{P}_{n-2}(\upsilon),$$

we finally get

$$s^{(n)} = -\frac{\sqrt{A}}{r}\,\frac{\widetilde{P}_n(\upsilon) - \lambda^{-2}\widetilde{P}_{n-2}(\upsilon)}{2n-1}, \quad n \geq 2, \tag{58}$$

to use in the discrete TBC:

$$(1 + R_e)\,\varphi_{J-1}^n - s^{(0)}\varphi_J^n = \sum_{k=1}^{n-1} s^{(n-k)}\varphi_J^k - (1 + R_e)\,\varphi_{J-1}^{n-1}, \quad n \geq 1. \tag{59}$$

Remark 12 *We see from* (57) *that for* $n \geq 2$ *the summed coefficients* $s^{(n)}$ *coincides with the convolution coefficients* (52) *for the implicit Euler scheme.*

Using a *recursion formula* for the scaled Legendre polynomials $\widetilde{P}_{n+1}(\upsilon) - \widetilde{P}_{n-1}(\upsilon)$:

$$\frac{\widetilde{P}_{n+1}(\upsilon) - \lambda^{-2}\widetilde{P}_{n-1}(\upsilon)}{2n+1} = \\ \upsilon\lambda^{-1}\frac{\widetilde{P}_{n}(\upsilon) - \lambda^{-2}\widetilde{P}_{n-2}(\upsilon)}{n+1} - \frac{n-2}{n+1}\lambda^{-2}\frac{\widetilde{P}_{n-1}(\upsilon) - \lambda^{-2}\widetilde{P}_{n-3}(\upsilon)}{2n-3}, \quad n \geq 2,$$

we see from (58) the *recurrence relation* for the summed convolution coefficients:

$$s^{(n+1)} = \frac{2n-1}{n+1}\upsilon\lambda^{-1}s^{(n)} - \frac{n-2}{n+1}\lambda^{-2}s^{(n-1)}, \quad n \geq 2, \tag{60}$$

which can be used after calculating $s^{(n)}$, $n = 0, 1, 2$ by the formula (57).

The starting coefficient of the recursion (cf. (49)) can be determined with

$$s^{(0)} = \ell^{(0)} = \lim_{z\to\infty} \nu_1(z) = \left(H + \frac{\kappa}{r}\right) + \frac{1+\sqrt{A}}{r}.$$

Here, the sign has to be fixed such that $|\nu_1(z)| > 1$ holds. This can be done for e.g. for $z = \infty$.

Ehrhardt proved in [22] that the problem of determining the required values of the convolution coefficients through the recurrence relation (60) is *well–conditioned* by applying partial results of the comprehensive article [23].

The rapid decay of the $s^{(n)} = \mathrm{O}(n^{-\frac{3}{2}})$ [22] motivates a *simplified discrete TBC* by restricting (59) to a convolution over the "recent past" (last M time levels):

$$(1 + P_e)\,\varphi_{J-1}^{n} - s^{(0)}\varphi_J^n = \sum_{k=n-M}^{n-1} s^{(n-k)}\varphi_J^k - (1 + P_e)\,\varphi_{J-1}^{n-1}, \quad n \geq 1. \tag{61}$$

We note that the stability of the resulting scheme is still not proven yet.

6.5 The Stability of the resulting Scheme

In this section we will prove the stability of the Crank–Nicolson scheme with the discrete TBC (59) and an appropriate discretization of the the boundary condition (3c):

$$D_h^+\varphi_0^{n+1/2} = \alpha\varphi_0^{n+1/2}, \qquad n \geq 0. \tag{62}$$

We consider for simplicity the scheme (36) with constant coefficients and $f_j^{n+1/2} = 0$ written in the form

$$\Delta_\tau^+\varphi_j^n = r\Delta_h^2\varphi_j^{n+1/2} - rP_e\Delta_h^-\varphi_j^{n+1/2} - 2\kappa u_j^{n+1/2}. \tag{63}$$

To use the *discrete energy method* we multiply (63) with $2\varphi_j^{n+1/2}$ and sum it up for the finite interior range $j = 1, 2, \ldots, J-1$, using *summation by parts*:

$$
\begin{aligned}
&\sum_{j=1}^{J-1} \Big[(\varphi_j^{n+1})^2 - (\varphi_j^n)^2\Big] \\
&\quad = 2r \sum_{j=1}^{J-1} \varphi_j^{n+1/2} \Delta_h^2 \varphi_j^{n+1/2} - 2r P_e \sum_{j=1}^{J-1} \varphi_j^{n+1/2} \Delta_h^- \varphi_j^{n+1/2} - 4\kappa \sum_{j=1}^{J-1} (\varphi_j^{n+1/2})^2 \\
&\quad = -2r \sum_{j=0}^{J-1} \Big(\Delta_h^+ \varphi_j^{n+1/2}\Big)^2 + 2r\varphi_J^{n+1/2} \Delta_h^- \varphi_J^{n+1/2} - 2r\varphi_0^{n+1/2} \Delta_h^+ \varphi_0^{n+1/2} \\
&\qquad - rP_e \sum_{j=1}^{J-1} \Big(\Delta_h^+ \varphi_j^{n+1/2}\Big)^2 - rP_e \Big(\varphi_1^{n+1/2}\Big)^2 + rP_e \Big(\varphi_J^{n+1/2}\Big)^2 \\
&\qquad - 2rP_e \varphi_J^{n+1/2} \varphi_{J-1}^{n+1/2} + 2rP_e \varphi_0^{n+1/2} \varphi_1^{n+1/2} - 4\kappa \sum_{j=1}^{J-1} (\varphi_j^{n+1/2})^2 \\
&\quad \le -2r\varphi_J^{n+1/2} [(1+P_e)\varphi_{J-1}^{n+1/2} - (1+\frac{P_e}{2})\varphi_J^{n+1/2}] \\
&\qquad - 2r[h\alpha + (1-h\alpha)^2] \Big(\varphi_0^{n+1/2}\Big)^2 .
\end{aligned}
$$

Finally a summation with respect to the index n yields the following estimate for the discrete L^2–norm (defined by $\|\varphi^n\|_2^2 := h \sum_{j=1}^{J-1} |\varphi_j^n|^2$)

$$
\begin{aligned}
\|\varphi^{N+1}\|_2^2 &\le \|\varphi^I\|_2^2 - \frac{2\mu\tau}{h} \sum_{n=0}^{N} \varphi_J^{n+1/2} \Big[(1+P_e)\varphi_{J-1}^{n+1/2} - (1+\frac{P_e}{2})\varphi_J^{n+1/2}\Big] \\
&\le \|\varphi^I\|_2^2 - \frac{2\mu\tau}{h} \sum_{n=0}^{N} \varphi_J^{n+1/2} \Big(\varphi_J^{n+1/2} * \tilde{\ell}^{(n)}\Big),
\end{aligned}
\tag{64}
$$

where $\tilde{\ell}^{(n)} := \ell^{(n)} - (1+\frac{P_e}{2})\delta_n^0$ is given in (48).

Again, as in the continuous case, it remains to show that the boundary–memory–term at $j = J$ in (64) is of *positive type*. To do so, we define the finite sequences

$$
f_n = \varphi_J^{n+1/2} * \tilde{\ell}^{(n)}, \quad g_n = \varphi_J^{n+1/2}, \qquad n = 0, 1, \ldots, N,
\tag{65}
$$

with $f_n = g_n = 0$ for $n > N$, i.e. $\sum_{n=0}^{N} f_n\, g_n \ge 0$ is to show. A $\mathcal{Z}$–transformation using the transformed discrete TBC (47) yields

$$
\begin{aligned}
\mathcal{Z}\{f_n\} = \hat{f}(z) &= \frac{z+1}{2}\, \hat{\varphi}_J^N(z) \Big[\nu_1(z) - (1+\frac{P_e}{2})\Big] \\
&= \frac{1}{2r}\, \hat{\varphi}_J^N(z) \Big\{\Big[z - 1 + \kappa(z+1)\Big] \pm \sqrt[+]{Az^2 - 2Bz + C}\Big\},
\end{aligned}
\tag{66}
$$

where $\hat{\varphi}_J^N(z) = \sum_{n=0}^{N} \varphi_J^n z^{-n}$ is analytic on $|z| > 0$. The zeros $z_{1,2}$ of the square root above are given by $z_{1,2} = \lambda^{-1}(\upsilon \pm \sqrt{\upsilon^2 - 1})$ with λ, υ defined in (51).

Typically we have $\lambda > 1$, $\upsilon > 1$ and it can be shown that $0 < z_2 < z_1 < 1$ holds. The expression above in the curly brackets is analytic for $|z| > z_1$ and continuous for $|z| \geq z_1$ and therefore $\hat{f}(z)$ is analytic on $|z| > z_1$. Note that we have to choose the sign in (66) such that it matches with $\nu_1(z)$ for $|z|$ sufficiently large. For the second sequence g_n we obtain

$$\mathcal{Z}\{g_n\} = \hat{g}(z) = \frac{z+1}{2}\,\hat{\varphi}_J^N(z), \tag{67}$$

i.e. $\hat{g}(z)$ is analytic on $|z| > 0$. Now the basic idea is to use *Plancherel's theorem* for the $\mathcal{Z}$–transformation:

Theorem 13 (Plancherel's Theorem [24]) *If $\hat{f}(z) = \mathcal{Z}\{f_n\}$ exists for $|z| > R_{\hat{f}} \geq 0$ and $\hat{g}(z) = \mathcal{Z}\{g_n\}$ for $|z| > R_{\hat{g}} \geq 0$ with $R_{\hat{f}}\,R_{\hat{g}} < 1$. Then there also exists $\mathcal{Z}\{f_n\,\bar{g}_n\}$ for $|z| > R_{\hat{f}}\,R_{\hat{g}}$ and the following relation holds:*

$$\sum_{n=0}^{\infty} f_n\,\bar{g}_n = \mathcal{Z}\{f_n\,\bar{g}_n\}(z=1) = \frac{1}{2\pi}\int_0^{2\pi} \hat{f}(r\,e^{i\xi})\,\overline{\hat{g}\Big(\frac{e^{i\xi}}{r}\Big)}\,d\xi.$$

The integration path is the circle $\mathcal{C}$ defined by $R_{\hat{f}} < r < 1/R_{\hat{g}}$ (if $R_{\hat{g}} = 0$: $R_{\hat{f}} < r < \infty$). Especially, if $R_{\hat{f}} < 1$, $R_{\hat{g}} < 1$ then $r = 1$ can be chosen to obtain:

$$\sum_{n=0}^{\infty} f_n\,\bar{g}_n = \frac{1}{2\pi}\int_0^{2\pi} \hat{f}(e^{i\xi})\,\overline{\hat{g}(e^{i\xi})}\,d\xi.$$

This theorem gives:

$$\begin{aligned}\sum_{n=0}^{N} f_n\,g_n &= \frac{1}{2\pi}\int_0^{2\pi} \hat{f}(z)\,\overline{\hat{g}(z)}\Big|_{z=e^{i\xi}}\,d\xi \\ &= \frac{1}{2\pi}\int_0^{\pi} \Big(\hat{f}(z)\,\overline{\hat{g}(z)} + \hat{f}(\bar{z})\,\overline{\hat{g}(\bar{z})}\Big)\Big|_{z=e^{i\xi}}\,d\xi \\ &= \frac{1}{\pi}\int_0^{\pi} \mathrm{Re}\,\Big\{\hat{f}(z)\,\overline{\hat{g}(z)}\Big\}\Big|_{z=e^{i\xi}}\,d\xi,\end{aligned}$$

where we have used the fact that $\hat{f}(\bar{z}) = \overline{\hat{f}(z)}$, $\hat{g}(\bar{z}) = \overline{\hat{g}(z)}$, since $f_n, g_n \in \mathbb{R}$. Using (66), (67) we obtain

$$\sum_{n=0}^{N} f_n\,g_n = \frac{1}{4\pi}\int_0^{\pi} |z+1|^2\,\left|\hat{\varphi}_J^N(z)\right|^2 \Big[\mathrm{Re}\,\{\nu_1(z)\} - \Big(1 + \frac{P_e}{2}\Big)\Big]\Big|_{z=e^{i\xi}}\,d\xi. \tag{68}$$

We remark that the pole of $\nu_1(z)$ at $z = -1$ is "cancelled" by $|z+1|^2$. From (68) we conclude that the discrete L^2–norm (64) is non–increasing in time if

$$\mathrm{Re}\,\{\nu_1(e^{i\xi})\} \geq 1 + \frac{P_e}{2}, \qquad \forall \xi \in [0, 2\pi], \tag{69}$$

holds. This property of ν_1 can be shown in the following way. On the unit circle $z = e^{i\xi}$, $0 \le \xi \le 2\pi$, we have $(z-1)/(z+1) = i\tan(\xi/2)$ and thereby

$$y(z) := \frac{1}{r}\Bigl(\frac{z-1}{z+1} + \kappa\Bigr) = \frac{1}{r}\Bigl(\kappa + i\tan\frac{\xi}{2}\Bigr), \qquad 0 \le \xi \le 2\pi.$$

Now $\nu_1(z)$ fulfils simply

$$\nu_1(z) - 1 - \frac{P_e}{2} = y(z) \pm \sqrt[+]{y(z)\bigl(2 + y(z)\bigr) + \frac{P_e^2}{4}}$$

and therefore we obtain the requested property

$$\mathrm{Re}\,\{\nu_1(z)\} - 1 - \frac{P_e}{2} = \frac{\kappa}{r} + \mathrm{Re}\Bigl\{\sqrt[+]{y(z)\bigl(2 + y(z)\bigr) + \frac{P_e^2}{4}}\Bigr\} \ge 0,$$

for $z = e^{i\xi}$, $0 \le \xi \le 2\pi$.

We then have the following *main result* of this section:

Theorem 14 *The numerical scheme* (63) *with the discrete TBC* (59) *and the boundary condition* (62) *is stable with the property:*

$$\|\varphi^{n+1}\|_h^2 := h \sum_{j=1}^{J-1} \Bigl(\varphi_j^{n+1}\Bigr)^2 \le \|\varphi^0\|_h^2, \quad n \ge 0. \tag{70}$$

Remark 15 *To remedy the deficiency that our discrete TBC is nonlocal in the time variable which is noticeable especially in long–time calculations one can construct a new approximative (local in time) transparent boundary condition using the approach [25]. This BC is an efficient convolution by an exponential approximation: only one simple update is needed in each time step to compute the discrete convolution. However, it is a priori not clear if the monotonicity property is retained with this approximative TBC.*

7 Numerical Example

In this section we want to compare the numerical results from using our *discrete TBC* (59) to the solution using either the *discretized TBC of Mayfield* (38) or the approximative *absorbing BC of Halpern* (42). Due to its construction, our discrete TBC yields exactly (up to round–off errors) the numerical half–space solution restricted to the finite computational interval and thus serves for an adequate discrete model for air pollution problems.

Example

In this example we consider the two–dimensional stationary problem (3) and used the parameters of the problem given in [5]:

$$u = 5, \quad w_g = 0.5, \quad \alpha = 0.1, \quad \sigma = 0,$$
$$\nu = 5, \quad Q = 10^4, \quad H = 100,$$

on the computational domain $z \in [0, 200]$ with the rather coarse grid $\tau = 10$ and $h = 5$ (which makes the difference in the accuracy more clear).

In the sequel we present the results when using the Crank–Nicolson scheme (25) based on the perturbed operator (19). Note that we have to employ forward differencing of the advection term for the stationary problem. We used the initial data (21) and the boundary condition (62) at the ground $z = 0$.

Figures 1 and 2 show some concentration profiles $\varphi(z)$, $\varphi(x)$, respectively. They are computed at different distances x from the source at $z = 100$ or at different heights z with the *discrete TBC* (59) applied at the artificial boundary $z = 200$.

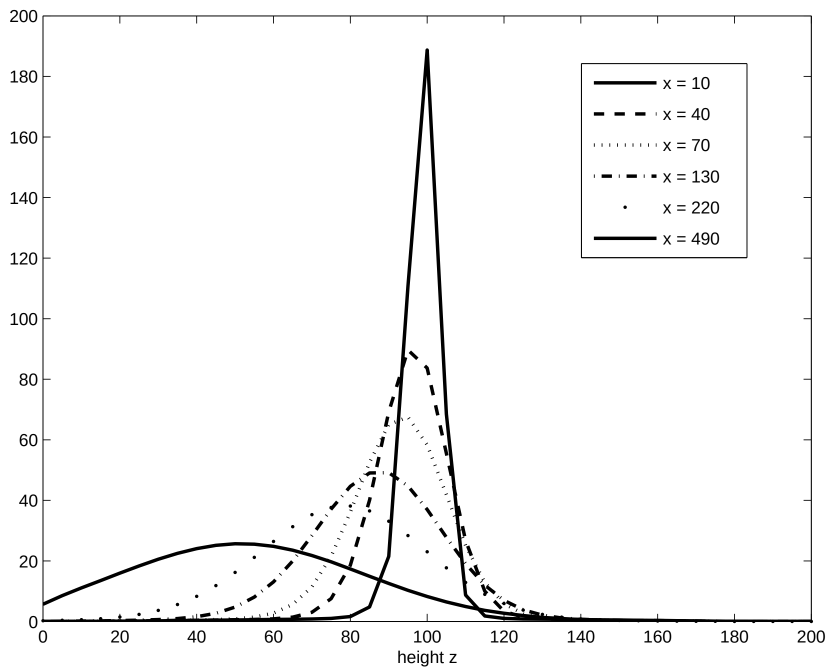

Fig. 1. Concentration profiles $\varphi(z)$ at different distances from the source at $z = 100$.

In Figure 3 the (negative) values of the summed coefficients $s^{(n)}$ are presented in a logarithmic plot. One clearly observes their rapid decay property which led to the idea of a *simplified discrete TBC* (59) by cutting off the discrete convolution after M terms.

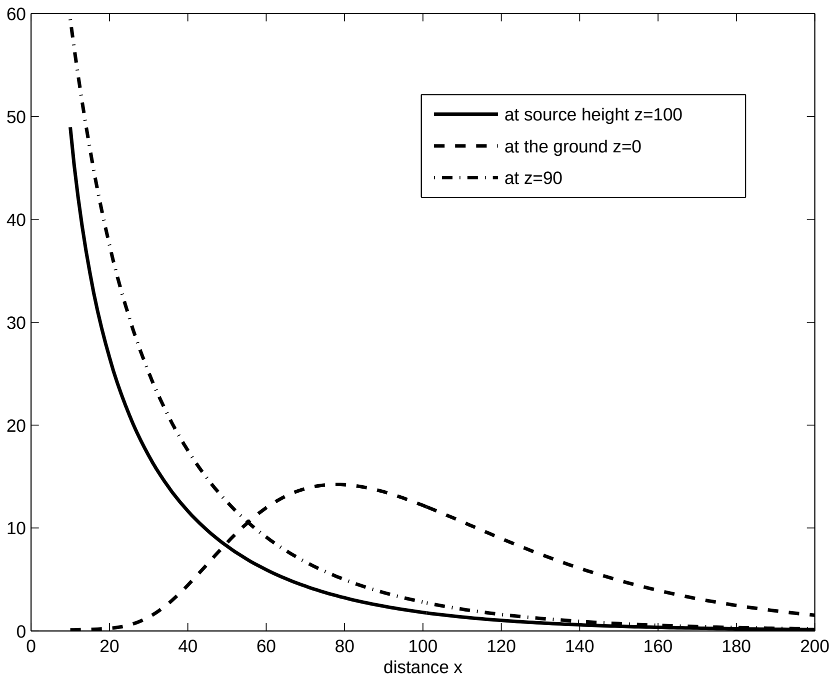

Fig. 2. Concentration profiles $\varphi(x)$ at different heights z.

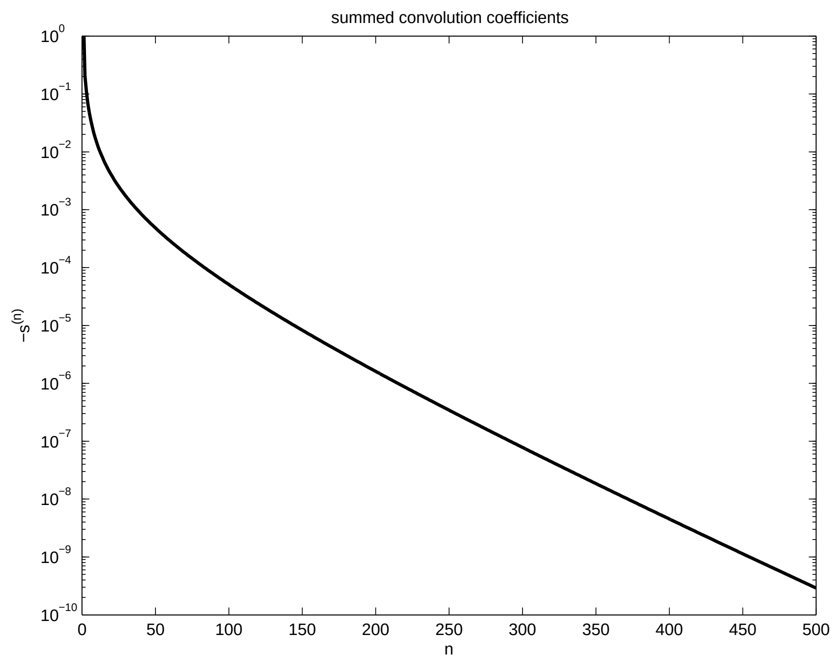

Fig. 3. Summed convolution coefficients $s^{(n)}$ for $n = 1, \ldots, 500$.

To measure the induced error (especially at the boundary) we calculate a *reference solution* on a three times larger domain (with a discrete TBC). The difference between the reference solution and the computed solution is called the *reflected part*. Figure 4 shows the *discrete* L^2*–norm* $\|\varphi^n\|_2 := (h \sum_{j=1}^{J-1} |\varphi_j^n|^2)^{1/2}$ of the reflected part computed with the discrete TBC (59) and in Figure 5 one can see the analogous results when using the boundary conditions of Mayfield and Halpern at $z = 200$. This illustrates the superiority of our *discrete TBC* (59) over both other strategies (observe the different scales!).

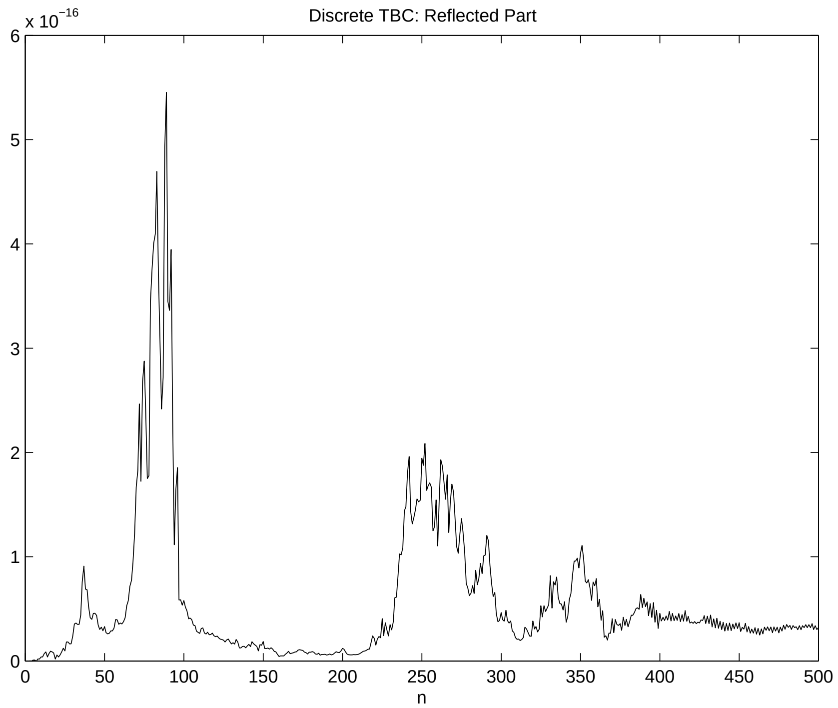

Fig. 4. Discrete TBC: L^2–norm of the reflected part (only roundoff–errors occur).

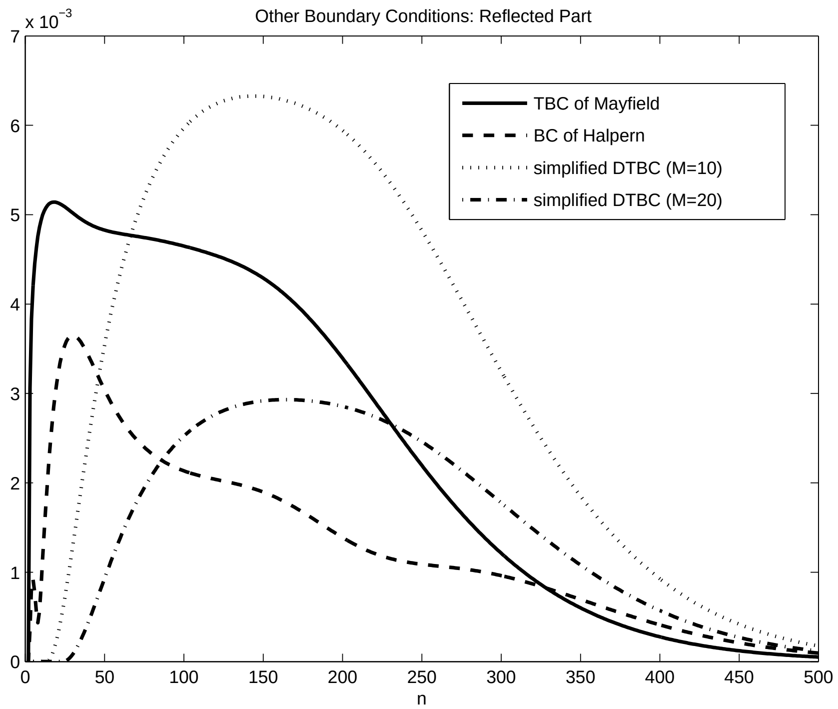

Fig. 5. Other Approaches: L^2–norm of the reflected part.

The simulation with the *discretized TBC* (38) from Mayfield requires the same numerical effort but the computed solution deviates (especially on coarse grids) from the half–space solution. The discretization of Mayfield is convergent (if a stability condition is fulfilled). The numerical results with the *first order boundary condition* (42) from Halpern are slightly better than the one with (38) but worse than the results with the *simplified discrete TBC* (61) with $M = 20$, which has comparable computational costs.

We emphasize the fact that the reflections due to the artificial boundary conditions (38), (42) are not that strong in this specific example taken from the literature [5]. This is due to the fact that only a very small amount of the concentration φ passes the artificial boundary at $z = 200$ (cf. Figure 1). However, if the computational domain is chosen smaller or if (for the transient problem (2)) the concentration is advected towards the artificial boundary, then the numerical reflections become much more apparent. Thus we reduce the computational domain to $z \in [0, 120]$ and plotted the corresponding results in Figure 6. The results are comparable to the ones shown in Figure 5. However, the magnitude of the error is now significantly larger and the peak of the error curve is reached earlier due to the smaller size of the domain. Finally we present in Figure 7 a comparison of the computational effort for the different approaches (for 10000 steps using the MATLAB function `cputime`). One observes that the Mayfield approach is even more costly than the exact discrete TBC and the computational cheapest artificial boundary condition in this example is the one of Halpern (42).

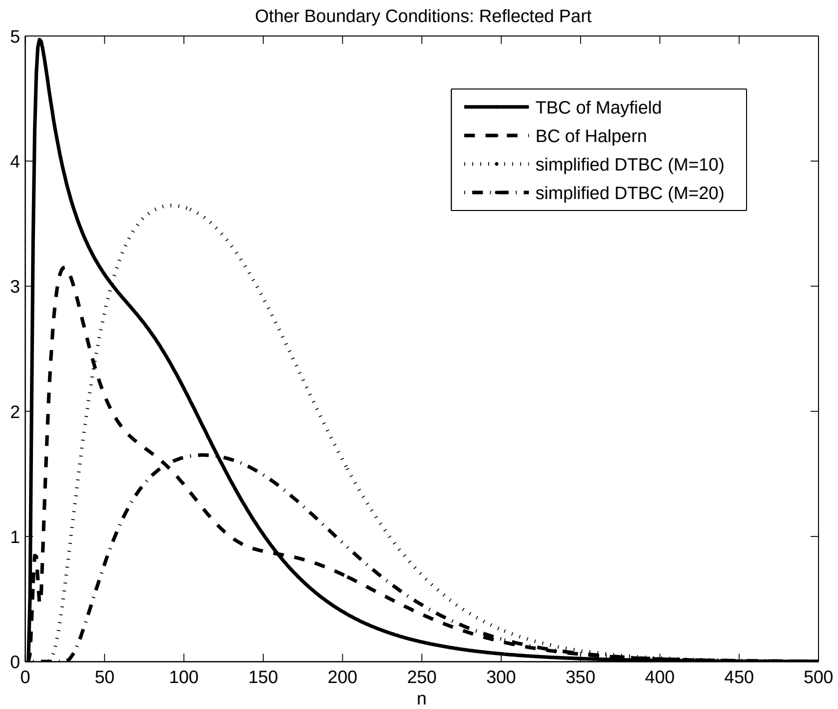

Fig. 6. L^2–norm of the reflected part for the reduced computational domain.

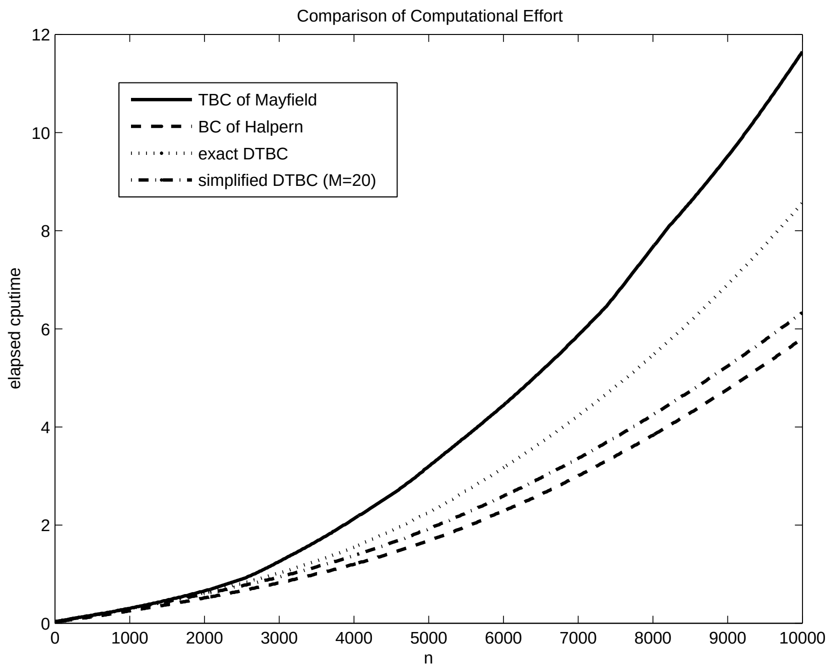

Fig. 7. Computational effort for the reduced computational domain and 10000 steps.

The reader is refered to [22, Chapter 2] for a detailed comparison study of the presented approaches for general advection–dffusion problems.

Conclusion

In this work we considered problems of air and water pollution. We discussed the concepts of monotonicity and positivity and presented adequate difference schemes that fulfill these requirements. For the numerical solution of an unbounded domain we constructed (discrete) transparent boundary conditions and proved the well–posedness of the analytic problem and the stability of the resulting scheme. Finally a numerical example showed the usefulness of our approach.

Future work will be concerned with nonuniform grids w.r.t. z, non–flat domains (mountains) and the propagation of active pollutants (e.g. ozone).

References

[1] M.E. Berljand, *Moderne Probleme der atmosphärischen Diffusion und der Verschmutzung der Atmosphäre*, Berlin, Akademie–Verlag, 1982.

[2] G.I. Marchuk, *Mathematical modelling in environmental problems*, Studies in mathematics and its applications 16, North–Holland, 1986.

[3] J.A. Cunge, F.M. Holly and A. Verwey, *Practical aspects of computational river hydraulics*, Pitman Pub. Inc., 1980.

[4] Nguyen Tat Dac, *One–Dimensional practical substance transport problems and their numerical procedures – Some applications*, Proc. of the 4th National conference on Gas and Fluid Mechanics, Hanoi, 1996, pp. 202-206 (Vietnamese).

[5] Dang Quang A and Ngo Van Luoc, *Numerical solution of a stationary problem of air pollution*, Proc. of NCST of Vietnam, **6** (1994), 11–23.

[6] Ngo Van Luoc, Dang Quang A and Nguyen Cong Dieu, *Analytic and Numerical solution of some problems of air pollution*, SEA Bull. Math. Special Issue, (1993), 105–117.

[7] A.A. Samarskii, *The theory of difference schemes*, Dekker, New York, 2001.

[8] N.N. Yanenko, *The method of fractional steps*, Springer–Verlag, 1971.

[9] H.Q. Wang and M. Lacroix, *Optimal weighting in the finite difference solution of the convection–dispersion equation*, Journal of hydrology **200** (1997), 228–242.

[10] Dang Quang A and Ngo Van Luoc, *Exact solution of a stationary problem of air pollution*, Proc. of the NCST of Vietnam **4** (1992), 39–46.

[11] J.C. Strikwerda, *Finite Difference Schemes and Partial Differential Equations*, Wadsworth & Brooks/Cole, 1989.

[12] H.-O. Kreiss and J. Lorenz, *Initial–Boundary Value Problems and the Navier–Stokes Equations*, Academic Press, 1989.

[13] G.I. Marchuk, *Methods of numerical mathematics*, Springer, New York, 1975.

[14] V.M. Paskonov, V.I. Polezhaev and L.A. Chudov, *Numerical modelling of heat and mass transfer*, Moscow, Nauka, 1984 (in Russian).

[15] K.O. Friedrichs, *Symmetric hyperbolic linear differential equations*, Comm. Pure Appl. Math. **7** (1954), 345–392.

[16] P. Matus, *The maximum principle and some of its applications*, Comput. Meth. in Appl. Math. **2** (2002), 50–91.

[17] B. Mayfield, *Non–local boundary conditions for the Schrödinger equation*, Ph.D. thesis, University of Rhode Island, Providence, RI, 1989.

[18] L. Halpern, *Artificial BC's for the Linear Advection Diffusion Equation*, Math. Comp. **46** (1986), 425–438.

[19] J.-P. Lohéac, *An Artificial Boundary Condition for an Advection–Diffusion Problem*, Math. Methods Appl. Sci. **14** (1991), 155–175.

[20] G. Lill, *Diskrete Randbedingungen an künstlichen Rändern*, Dissertation, Technische Hochschule Darmstadt, 1992.

[21] M. Ehrhardt, *Discrete Transparent Boundary Conditions for Parabolic Equations*, Z. Angew. Math. Mech. **77** (1997) S2, 543–544.

[22] M. Ehrhardt. *Discrete Artificial Boundary Conditions*, Ph.D. Thesis, Technische Universität Berlin, 2001.

[23] W. Gautschi, *Computational aspects of three–term recurrence relations*, SIAM Rev. **9** (1967), 24–82.

[24] G. Doetsch, *Anleitung zum praktischen Gebrauch der Laplace-Transformation und der Z-Transformation*, R. Oldenburg Verlag München, Wien, 3. Auflage 1967.

[25] A. Arnold, M. Ehrhardt and I. Sofronov, *Discrete transparent boundary conditions for the Schrödinger equation: Fast calculation, approximation, and stability*, Comm. Math. Sci. **1** (2003), 501–556.