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The Complete Flux Scheme for Conservation Laws in Curvilinear Coordinates

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1. Introduction

Conservation laws are ubiquitous in continuum physics, they occur in disciplines like fluid mechanics, combustion theory, plasma physics, etc. These conservation laws are often of advection-diffusion-reaction type, describing the interplay between different processes such as advection or drift, diffusion or conduction and chemical reactions or ionization. Examples are the conservation equations for reacting flow [8] or plasmas [9]. Sometimes, these conservation laws hold in spherical or cylindrical geometries, and in such cases it is convenient to reformulate the conservation laws in the corresponding coordinate system. In combustion theory, for example, the study of spherical and cylindrical flames is useful for finding parameters such as burning velocity or flame curvature [1].

For space discretization of these conservation laws we consider the finite volume method in combination with the complete flux scheme to approximate the fluxes at the cell interfaces. The complete flux scheme for Cartesian coordinates is introduced in [13]. The purpose of this contribution is to generalize the complete flux scheme to conservation laws in spherical or cylindrical coordinates.

The development of the complete flux scheme is inspired by papers by Thiart [10, 11]. The basic idea of the complete flux scheme is to compute the numerical flux at a cell interface from a local (one-dimensional) boundary value problem for the *entire* equation, including the source term. As such, the scheme is a generalization of the exponential scheme, where the flux is determined from a local, constant coefficient, homogeneous equation [4, 6]. Our approach is to first derive an integral representation for the flux, and subsequently apply suitable quadrature rules to obtain the numerical flux. As a consequence, the numerical flux is the superposition of a homogeneous and inhomogeneous flux, corresponding to the advection-diffusion operator and the source term, respectively. The resulting discretization has a three-point coupling in each spatial direction, shows uniform second order convergence and virtually never generates spurious oscillations [13]. The purpose of this chapter is to extend this approach to conservation laws, where the advection-diffusion operation is formulated in spherical or cylindrical coordinates. Another important issue is the extension to time-dependent problems. The key idea is then to consider the time derivative as a source

term, and to include it in the inhomogeneous flux. The resulting implicit ODE system often has small dissipation and dispersion errors [15].

We have organised our paper as follows. The finite volume method for conservation laws in spherical and cylindrical coordinates is outlined in Section 2. In Section 3 we briefly repeat the complete flux scheme for stationary, one-dimensional conservation laws in Cartesian coordinates. The extension to spherical coordinates is presented in Section 4, and the next logical extension to cylindrical coordinates, is discussed in Section 5. How to deal with time dependent conservation laws is demonstrated in Section 6 for spherical coordinates. As an example, we present in Section 7 the numerical solution of a premixed, spherical flame, and finally in Section 8, we give a summary and formulate conclusions.

2. Finite volume discretization

In this section we outline the finite volume method (FVM) for a generic conservation law of advection-diffusion-reaction type, defined on a domain in R^d $(d = 1, 2, 3)$. Therefore, consider the following model equation

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot (\boldsymbol{u}\varphi - \varepsilon \nabla \varphi) = s, \tag{2.1}$$

where $\boldsymbol{u}$ is a mass flux or (drift) velocity, $\varepsilon \geq \varepsilon_{\min} > 0$ a diffusion coefficient, and s a source term describing, e.g., chemical reactions or ionization. The unknown φ is then the mass fraction of one of the constituent species in a chemically reacting flow or a plasma. The parameters ε and s are usually (complicated) functions of φ whereas the vector field $\boldsymbol{u}$ has to be computed from (flow) equations corresponding to (2.1). However, for the sake of discretization, we will consider these parameters as given functions of the spatial coordinates $\boldsymbol{x}$ and the time t. Moreover, in the derivation of the numerical flux, we assume that the vector field $\boldsymbol{u}$ is incompressible, i.e.,

$$\nabla \cdot \boldsymbol{u} = 0. \tag{2.2}$$

Equation (2.1) is a prototype of a conservation law for a mixture, defining the mass balance for φ, and equation (2.2) is a simplified version of the corresponding continuity equation, describing conservation of mass or charge in the mixture.

Associated with equation (2.1) we introduce the flux vector $\boldsymbol{f}$, defined by

$$\boldsymbol{f} := \boldsymbol{u}\varphi - \varepsilon \nabla \varphi. \tag{2.3}$$

Consequently, equation (2.1) can be concisely written as $\partial\varphi/\partial t + \nabla \cdot \boldsymbol{f} = s$. Integrating this equation over a fixed domain $\Omega \subset \mathrm{R}^d$ and applying Gauss' theorem we obtain the integral form of the conservation law, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \varphi \, \mathrm{d}V + \oint_\Gamma \boldsymbol{f} \cdot \boldsymbol{n} \, \mathrm{d}S = \int_\Omega s \, \mathrm{d}V, \tag{2.4}$$

where $\boldsymbol{n}$ is the outward unit normal on the boundary $\Gamma = \partial\Omega$. This equation is the basic conservation law, which reduces to (2.1) provided φ is smooth enough.

In the FVM we cover the domain with a finite number of disjunct control volumes or cells $\Omega_{\mathtt{j}}$ and impose the integral form (2.4) for each of these cells. The index $\mathtt{j}$ is an index vector for multi-dimensional problems. We restrict ourselves to uniform tensor product grids for an orthogonal, curvilinear coordinate system $\boldsymbol{\xi} = (\xi^1, \xi^2, \xi^3)$ and adopt the vertex-centred approach [16], i.e., we first choose the grid points $\boldsymbol{\xi}_{\mathtt{j}} = (\xi^1_j, \xi^2_k, \xi^3_l)$ with $\mathtt{j} = (j,k,l)$, where the unknown φ has to be approximated and subsequently choose the control volume $\Omega_{\mathtt{j}} = [\xi^1_{j-1/2}, \xi^1_{j+1/2}] \times [\xi^2_{k-1/2}, \xi^2_{k+1/2}] \times [\xi^3_{l-1/2}, \xi^3_{l+1/2}]$ with $\xi^1_{j\pm1/2} := \frac{1}{2}(\xi^1_j + \xi^1_{j\pm1})$ etc. The boundary $\Gamma_{\mathtt{j}} = \partial\Omega_{\mathtt{j}}$ is then the union of six interface surfaces $\Gamma_{\mathtt{j},\mathtt{j}\pm\mathtt{e}^i} (i = 1,2,3)$ where, e.g., $\Gamma_{\mathtt{j},\mathtt{j}+\mathtt{e}^1} := \{\xi^1_{j+1/2}\} \times [\xi^2_{k-1/2}, \xi^2_{k+1/2}] \times [\xi^3_{l-1/2}, \xi^3_{l+1/2}]$ is the interface through $(\xi^1_{j+1/2}, \xi^2_k, \xi^3_l)$ and perpendicular to the line segment connecting $\xi_{\mathtt{j}}$ and $\xi_{\mathtt{j}+\mathtt{e}^1}$. The (integral) conservation law for such a control volume reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_{\mathtt{j}}} \varphi \,\mathrm{d}V + \sum_{\mathtt{k}\in\mathcal{N}(\mathtt{j})} \int_{\Gamma_{\mathtt{j},\mathtt{k}}} \boldsymbol{f}\cdot\boldsymbol{n} \,\mathrm{d}S = \int_{\Omega_{\mathtt{j}}} s \,\mathrm{d}V, \tag{2.5}$$

where $\mathcal{N}(\mathtt{j}) = \{\mathtt{j} \pm \mathtt{e}^i \mid i = 1,2,3\}$ is the index set of neighbouring grid points of $\boldsymbol{\xi}_{\mathtt{j}}$ and where $\Gamma_{\mathtt{j},\mathtt{k}}$ is the face of the boundary $\Gamma_{\mathtt{j}}$ connecting the adjacent cells $\Omega_{\mathtt{j}}$ and $\Omega_{\mathtt{k}}$. The unit normal $\boldsymbol{n}$ on $\Gamma_{\mathtt{j},\mathtt{k}}$ is directed from $\boldsymbol{\xi}_{\mathtt{j}}$ to $\boldsymbol{\xi}_{\mathtt{k}}$. Obviously, the volume element $\mathrm{d}V$ and the surface elements $\mathrm{d}S$ have to be expressed in terms of the curvilinear coordinates $\boldsymbol{\xi}$. Approximating the volume and surface integrals in (2.5) by the midpoint rule, we obtain the following semi-discrete conservation law for $\varphi_{\mathtt{j}}(t) \approx \varphi(\boldsymbol{\xi}_{\mathtt{j}}, t)$, i.e.,

$$\dot{\varphi}_{\mathtt{j}}(t) V_{\mathtt{j}} + \sum_{\mathtt{k}\in\mathcal{N}(\mathtt{j})} (\boldsymbol{F}\cdot\boldsymbol{n})_{\mathtt{j},\mathtt{k}} A_{\mathtt{j},\mathtt{k}} = s_{\mathtt{j}}(t) V_{\mathtt{j}}, \tag{2.6}$$

where $V_{\mathtt{j}}$ is the volume of $\Omega_{\mathtt{j}}$, $A_{\mathtt{j},\mathtt{k}}$ the area of $\Gamma_{\mathtt{j},\mathtt{k}}$, $\dot{\varphi}_{\mathtt{j}}(t) \approx \partial\varphi/\partial t(\boldsymbol{\xi}_{\mathtt{j}}, t)$ and $s_{\mathtt{j}}(t) = s(\boldsymbol{\xi}_{\mathtt{j}}, t)$. Furthermore, $(\boldsymbol{F}\cdot\boldsymbol{n})_{\mathtt{j},\mathtt{k}}$ is the normal component on $\Gamma_{\mathtt{j},\mathtt{k}}$, at the interface point $\boldsymbol{\xi}_{\mathtt{j},\mathtt{k}} := \frac{1}{2}(\boldsymbol{\xi}_{\mathtt{j}} + \boldsymbol{\xi}_{\mathtt{k}})$ of the numerical flux vector $\boldsymbol{F}$, approximating $(\boldsymbol{f}\cdot\boldsymbol{n})(\boldsymbol{\xi}_{\mathtt{j},\mathtt{k}}, t)$. Obviously, for stationary problems the time derivatives in (2.5) and (2.6) can be discarded.

In this paper we consider the formulation of the conservation law (2.1) in terms of the spherical coordinates (r,ϕ,θ) and the cylindrical coordinates (r,θ,z). In the first case, we assume spherical symmetry, i.e., $\varphi = \varphi(r,t)$ and $\boldsymbol{f} = f(r,t)\boldsymbol{e}_r$. As a typical example we mention a spherical flame; see Section 7. A control volume is then given by the spherical shell $\Omega_j = [r_{j-1/2}, r_{j+1/2}] \times [0,\pi] \times [0,2\pi)$ and the surface integral over $\Gamma_j = \partial\Omega_j$ can be written as

$$\begin{aligned}\oint_{\Gamma_j} \boldsymbol{f}\cdot\boldsymbol{n} \,\mathrm{d}S &= \int_{r=r_{j+1/2}} \boldsymbol{f}\cdot\boldsymbol{e}_r \,\mathrm{d}S - \int_{r=r_{j-1/2}} \boldsymbol{f}\cdot\boldsymbol{e}_r \,\mathrm{d}S \\ &= 4\pi\big(r^2_{j+1/2} f(r_{j+1/2},t) - r^2_{j-1/2} f(r_{j-1/2},t)\big),\end{aligned} \tag{2.7}$$

where we used the shorthand notation $r = r_{j+1/2}$ to denote the sphere $\{r_{j+1/2}\} \times [0,\pi] \times [0,2\pi)$. Note that this expression for the surface integral of the flux is exact and replaces the second term in (2.5). For the approximation of the volume integrals in (2.5) we apply the midpoint rule, so we find

$$\int_{\Omega_j} s \,\mathrm{d}V \doteq \tfrac{4}{3}\pi\big(r^3_{j+1/2} - r^3_{j-1/2}\big)\, s_j(t). \tag{2.8}$$

Combining (2.5), (2.7) and (2.8) and using the relation $x^3 - y^3 = (x-y)(x^2+xy+y^2)$ we obtain the semidiscrete conservation law

$$\Delta r\big(r_j^2 + \tfrac{1}{12}\Delta r^2\big)\,\dot{\varphi}_j(t) + r_{j+1/2}^2 F_{j+1/2}(t) - r_{j-1/2}^2 F_{j-1/2}(t) = \Delta r\big(r_j^2 + \tfrac{1}{12}\Delta r^2\big)\,s_j(t), \tag{2.9}$$

where $F_{j+1/2}(t)$ denotes the numerical flux approximating $f(r_{j+1/2},t)$ etc..

Next, for cylindrical coordinates, we assume cylindrical symmetry, i.e., $\varphi = \varphi(r,z,t)$ and $\boldsymbol{f} = \boldsymbol{f}_r(r,z,t)\boldsymbol{e}_r + \boldsymbol{f}_z(r,z,t)\boldsymbol{e}_z$. In this case a control volume is the cylindrical shell $\Omega_{j,l} = [r_{j-1/2}, r_{j+1/2}] \times [0,2\pi) \times [z_{l-1/2}, z_{l+1/2}]$. The surface integral of the flux over the boundary $\Gamma_{j,l} = \partial\Omega_{j,l}$ contains four terms and is given by

$$\begin{aligned}\oint_{\Gamma_{j,l}} \boldsymbol{f}\cdot\boldsymbol{n}\,\mathrm{d}S &= \int_{r=r_{j+1/2}} f_r\,\mathrm{d}S - \int_{r=r_{j-1/2}} f_r\,\mathrm{d}S + \int_{z=z_{l+1/2}} f_z\,\mathrm{d}S - \int_{z=z_{l-1/2}} f_z\,\mathrm{d}S \\ &\doteq 2\pi\Delta z\big(r_{j+1/2} f_{r,j+1/2,l}(t) - r_{j-1/2} f_{r,j-1/2,l}(t)\big) + \\ &\quad 2\pi\Delta r\, r_j\big(f_{z,j,l+1/2}(t) - f_{z,j,l-1/2}(t)\big),\end{aligned} \tag{2.10}$$

where for example $r = r_{j+1/2}$ denotes the interface $\{r_{j+1/2}\} \times \big[0,2\pi\big) \times \big[z_{l-1/2}, z_{l+1/2}\big]$, and likewise for all other interfaces. For the approximation of the volume integrals in (2.5) we use once more the midpoint rule, giving the approximation

$$\int_{\Omega_{j,l}} s\,\mathrm{d}V \doteq 2\pi\Delta r\Delta z\, r_j s_{j,l}(t). \tag{2.11}$$

Analogous to the previous case, combining (2.5), (2.10) and (2.11) we obtain the semidiscrete conservation law

$$\begin{aligned}&\Delta r\Delta z\, r_j\,\dot{\varphi}_{j,l}(t) + \Delta z\big(r_{j+1/2}F_{r,j+1/2,l}(t) - r_{j-1/2}F_{r,j-1/2,l}(t)\big) + \\ &\quad \Delta r\, r_j\big(F_{z,j,l+1/2}(t) - F_{z,j,l-1/2}(t)\big) = \Delta r\Delta z\, r_j\, s_{j,l}(t),\end{aligned} \tag{2.12}$$

where $F_{r,j+1/2,l}(t)$ is the numerical flux approximating $f_r(r_{j+1/2}, z_l, t)$ and likewise for $F_{z,j,l+1/2}(t)$. In the following we suppress the explicit dependence on t.

The FVM has to be completed with expressions for the numerical flux. We require that $(\boldsymbol{F}\cdot\boldsymbol{n})_{\mathtt{j},\mathtt{k}}$ depends on φ and a modified source term $\tilde{s}$ in the neighbouring grid points $\boldsymbol{x}_\mathtt{j}$ and $\boldsymbol{x}_\mathtt{k}$, i.e., we are looking for an expression of the form

$$(\boldsymbol{F}\cdot\boldsymbol{n})_{\mathtt{j},\mathtt{k}} = \alpha_{\mathtt{j},\mathtt{k}}\varphi_\mathtt{j} - \beta_{\mathtt{j},\mathtt{k}}\varphi_\mathtt{k} + d_{\mathtt{j},\mathtt{k}}\big(\gamma_{\mathtt{j},\mathtt{k}}\tilde{s}_\mathtt{j} + \delta_{\mathtt{j},\mathtt{k}}\tilde{s}_\mathtt{k}\big), \tag{2.13}$$

where $d_{\mathtt{j},\mathtt{k}} := |\boldsymbol{x}_\mathtt{j} - \boldsymbol{x}_\mathtt{k}|$. The variable $\tilde{s}$ includes the source term and an additional terms like the cross flux or time derivative, when appropriate. The derivation of expressions for the numerical flux is detailed in the next sections.

3. Numerical flux for Cartesian coordinates

In this section we outline the derivation of the complete flux scheme for the steady, one-dimensional conservation laws in Cartesian coordinates, which is based on the integral representation of the flux. The derivation is a summary of the theory in [3, 13].

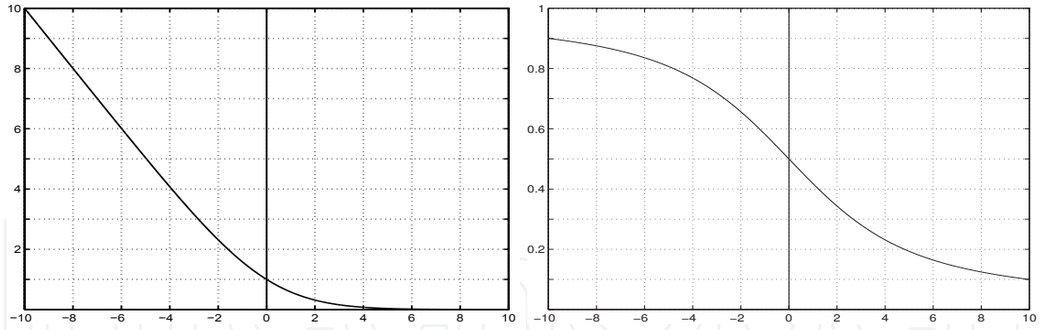

Fig. 1. The Bernoulli function B (left) and the function W (right).

The conservation law can be written as $\mathrm{d}f/\mathrm{d}x = s$ with $f = u\varphi - \varepsilon\,\mathrm{d}\varphi/\mathrm{d}x$. The integral representation of the flux $f_{j+1/2} := f(x_{j+1/2})$ at the cell edge $x_{j+1/2}$ located between the grid points x_j and x_{j+1} is based on the following model boundary value problem (BVP) for the variable φ:

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big(u\varphi - \varepsilon\frac{\mathrm{d}\varphi}{\mathrm{d}x}\Big) = s, \quad x_j < x < x_{j+1}, \tag{3.1a}$$

$$\varphi(x_j) = \varphi_j, \quad \varphi(x_{j+1}) = \varphi_{j+1}. \tag{3.1b}$$

In accordance with (2.13), we derive an expression for the flux $f_{j+1/2}$ corresponding to the solution of the *inhomogeneous* BVP (3.1), implying that $f_{j+1/2}$ not only depends on u and ε, but also on the source term s. It is convenient to introduce the variables a, P, A and S for $x \in (x_j, x_{j+1})$ by

$$a := \frac{u}{\varepsilon}, \quad P := a\Delta x, \quad A(x) := \int_{x_{j+1/2}}^{x} a(\xi)\,\mathrm{d}\xi, \quad S(x) := \int_{x_{j+1/2}}^{x} s(\xi)\,\mathrm{d}\xi. \tag{3.2}$$

Here, P and A are the Peclet function and Peclet integral, respectively, generalizing the well-known (numerical) Peclet number. Integrating the differential equation $\mathrm{d}f/\mathrm{d}x = s$ from $x_{j+1/2}$ to $x \in (x_j, x_{j+1})$ we get the integral balance $f(x) - f_{j+1/2} = S(x)$. Using the definition of A in (3.2), it is clear that the flux can be rewritten as $f = -\varepsilon\,\mathrm{e}^{A}\,\mathrm{d}\big(\mathrm{e}^{-A}\,\varphi\big)/\mathrm{d}x$. Substituting this into the integral balance, isolating the derivative $\mathrm{d}\big(\mathrm{e}^{-A}\varphi\big)/\mathrm{d}x$, and integrating from x_j to x_{j+1} we obtain the following expressions for the flux:

$$f_{j+1/2} = f^{\mathrm{h}}_{j+1/2} + f^{\mathrm{i}}_{j+1/2}, \tag{3.3a}$$

$$f^{\mathrm{h}}_{j+1/2} = \big(\mathrm{e}^{-A_j}\varphi_j - \mathrm{e}^{-A_{j+1}}\varphi_{j+1}\big) \Big/ \int_{x_j}^{x_{j+1}} \varepsilon^{-1}\mathrm{e}^{-A}\,\mathrm{d}x, \tag{3.3b}$$

$$f^{\mathrm{i}}_{j+1/2} = -\int_{x_j}^{x_{j+1}} \varepsilon^{-1}\mathrm{e}^{-A}S\,\mathrm{d}x \Big/ \int_{x_j}^{x_{j+1}} \varepsilon^{-1}\mathrm{e}^{-A}\,\mathrm{d}x, \tag{3.3c}$$

where $f^{\mathrm{h}}_{j+1/2}$ and $f^{\mathrm{i}}_{j+1/2}$ are the homogeneous and inhomogeneous part, corresponding to the homogeneous and particular solution of (3.1), respectively.

In the following we assume that u and ε are constant; extension to variable coefficients is discussed in [3, 13]. In this case we can determine all integrals involved. Moreover,

substituting the expression for $S(x)$ in (3.3c) and changing the order of integration, we can derive an alternative expression for the inhomogeneous flux. This way we obtain

$$f^{\mathrm{h}}_{j+1/2} = \frac{\varepsilon}{\Delta x}\big(B(-P)\varphi_j - B(P)\varphi_{j+1}\big), \tag{3.4a}$$

$$f^{\mathrm{i}}_{j+1/2} = \Delta x \int_0^1 G(\sigma; P, \sigma_{j+1/2}) s(x(\sigma))\,\mathrm{d}\sigma, \quad x(\sigma) = x_j + \sigma\Delta x. \tag{3.4b}$$

Here $B(z) := z/\big(\mathrm{e}^z - 1\big)$ is the generating function of the Bernoulli numbers, in short Bernoulli function, see Figure 1, $P := u\Delta x/\varepsilon$ is the Peclet number, and $G = G(\sigma; P, \sigma_{\mathrm{b}})$ is the Green's function for the flux, given by

$$G(\sigma; P, \sigma_{\mathrm{b}}) := \begin{cases} \dfrac{1 - \mathrm{e}^{-P\sigma}}{1 - \mathrm{e}^{-P}} & \text{for} \quad 0 \le \sigma \le \sigma_{\mathrm{b}}, \\[2ex] -\dfrac{1 - \mathrm{e}^{P(1-\sigma)}}{1 - \mathrm{e}^{P}} & \text{for} \quad \sigma_{\mathrm{b}} < \sigma \le 1, \end{cases} \tag{3.5}$$

see Figure 2. Note that G relates the *flux* to the source term and is different from the usual Green's function, which relates the *solution* to the source term. G is a function of the normalized coordinate $\sigma = (x - x_j)/\Delta x$ $(0 \le \sigma \le 1)$ between x_j and x_{j+1} and depends on the parameters P and σ_{b}, the σ-coordinate of the cell boundary. Obviously, $\sigma_{j+1/2} = \sigma\big(x_{j+1/2}\big) = \frac{1}{2}$. For the constant coefficient homogeneous flux we introduce the function

$$f^{\mathrm{h}}_{j+1/2} = \mathcal{F}^{\mathrm{h}}\big(\varepsilon/\Delta x, P; \varphi_j, \varphi_{j+1}\big) := \frac{\varepsilon}{\Delta x}\big(B(-P)\varphi_j - B(P)\varphi_{j+1}\big), \tag{3.6}$$

to denote the dependence of $f^{\mathrm{h}}_{j+1/2}$ on the parameter values $\varepsilon/\Delta x$ and P and on the function values φ_j and φ_{j+1}; cf. (2.13). The homogeneous flux (3.6) is the well-known exponential flux [7].

Next, we give the numerical flux $F_{j+1/2}$. For the homogeneous component $F^{\mathrm{h}}_{j+1/2}$ we obviously take (3.6), i.e., $F^{\mathrm{h}}_{j+1/2} = \mathcal{F}^{\mathrm{h}}\big(\varepsilon/\Delta x, P; \varphi_j, \varphi_{j+1}\big)$. The approximation of the inhomogeneous component $f^{\mathrm{i}}_{j+1/2}$ depends on P. For dominant diffusion ($|P| \ll 1$) the average value of $G(\sigma; P)$ is small, which implies that the inhomogeneous flux is of little importance. On the contrary, for dominant advection ($|P| \gg 1$), the average value of $G(\sigma; P)$

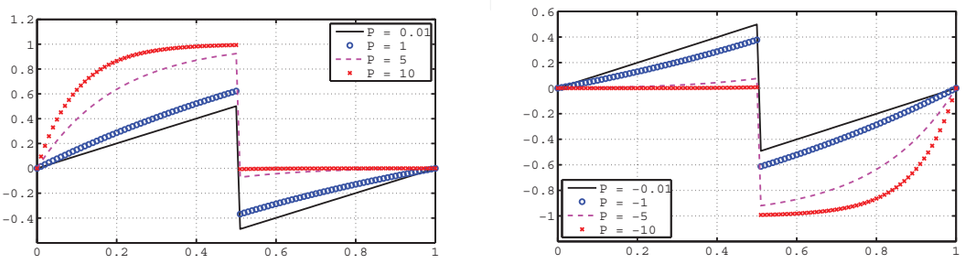

Fig. 2. Green's function for the flux for $P > 0$ (left) and $P < 0$ (right).

on the half interval upwind of $\sigma = \frac{1}{2}$, i.e., the interval $[0, \frac{1}{2}]$ for $u > 0$ and $[\frac{1}{2}, 1]$ for $u < 0$, is much larger than the average value on the downwind half. This means that for dominant advection the upwind value of s is the relevant one, and therefore we replace $s(x(\sigma))$ in (3.4b) by its upwind value $s_{\mathrm{u},j+1/2}$, i.e., $s_{\mathrm{u},j+1/2} = s_j$ if $u \geq 0$ and $s_{\mathrm{u},j+1/2} = s_{j+1}$ if $u < 0$, and evaluate the resulting integral exactly. This way we obtain

$$F_{j+1/2} = \mathcal{F}^{\mathrm{h}}\big(\varepsilon/\Delta x, P; \varphi_j, \varphi_{j+1}\big) + \Delta x \left(\tfrac{1}{2} - W(P)\right) s_{\mathrm{u},j+1/2}, \tag{3.7}$$

where $W(z) := \big(\mathrm{e}^z - 1 - z\big)/\big(z\big(\mathrm{e}^z - 1\big)\big)$; see Figure 1. From this expression it is once more clear that the inhomogeneous component is only of importance for dominant advection. We refer to (3.7) as the complete flux (CF) scheme, as opposed to the homogeneous flux (HF) scheme for which we omit the inhomogeneous component.

4. Numerical flux for spherical coordinates

Our objective in this section is to extend the derivation in the previous section to spherical coordinates, assuming spherical symmetry.

The stationary conservation law can be written as $\mathrm{d}\big(r^2 f\big)/\mathrm{d}r = r^2 s$ with $f = u\varphi - \varepsilon \mathrm{d}\varphi/\mathrm{d}r$. The expression for the flux $f_{j+1/2} := f(r_{j+1/2})$ at the cell boundary $r_{j+1/2}$ is based on the following model BVP for the unknown φ:

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\Big(r^2\Big(u\varphi - \varepsilon\frac{\mathrm{d}\varphi}{\mathrm{d}r}\Big)\Big) = s, \quad r_j < r < r_{j+1}, \tag{4.1a}$$

$$\varphi(r_j) = \varphi_j, \quad \varphi(r_{j+1}) = \varphi_{j+1}, \tag{4.1b}$$

where ε and s are sufficiently smooth functions of r. Moreover, we assume that $u > 0$ and, in view of (2.2), u satisfies the relation

$$U := r^2 u = \text{Const} \quad \text{for} \quad r \in (r_j, r_{j+1}). \tag{4.2}$$

Analogous to the flux in Cartesian coordinates, we derive an integral relation for the flux that is the superposition of the homogeneous flux, depending on the advection-diffusion operator, and the inhomogeneous flux, taking into account the effect of the source term s. Approximating all integrals involved gives us the expression for the numerical flux $F_{j+1/2}$.

Analogous to (3.2) we introduce the variables D, a, P, A and S, defined by

$$\begin{aligned} &D := r^2\,\varepsilon, \quad a := \frac{U}{D}, \quad P := a\Delta r, \\ &A(r) := \int_{r_{j+1/2}}^{r} a(\eta)\,\mathrm{d}\eta, \quad S(r) := \int_{r_{j+1/2}}^{r} \eta^2 s(\eta)\,\mathrm{d}\eta. \end{aligned} \tag{4.3}$$

We refer to P and A as the Peclet function and Peclet integral, respectively. Integrating the conservation law from $r_{j+1/2}$ to $r \in (r_j, r_{j+1})$, we obtain the relation

$$r^2 f(r) - \big(r^2 f\big)(r_{j+1/2}) = S(r). \tag{4.4}$$

Using the definitions of D and A in (4.3), it is clear that the expression for the flux can be rewritten as

$$r^2 f = U\varphi - D\frac{\mathrm{d}\varphi}{\mathrm{d}r} = -D\,\mathrm{e}^{A}\frac{\mathrm{d}}{\mathrm{d}r}\left(\varphi\,\mathrm{e}^{-A}\right). \tag{4.5}$$

Inserting this expression in (4.4), isolating the derivative $\mathrm{d}\left(\varphi\,\mathrm{e}^{-A}\right)/\mathrm{d}r$, and integrating the resulting equation from r_j to r_{j+1} we obtain the following expressions for the flux:

$$\left(r^2 f\right)_{j+1/2} = \left(r^2 f^{\mathrm{h}}\right)_{j+1/2} + \left(r^2 f^{\mathrm{i}}\right)_{j+1/2}, \tag{4.6a}$$

$$\left(r^2 f^{\mathrm{h}}\right)_{j+1/2} = \left(\mathrm{e}^{-A_j}\varphi_j - \mathrm{e}^{-A_{j+1}}\varphi_{j+1}\right) \Big/ \int_{r_j}^{r_{j+1}} D^{-1}\mathrm{e}^{-A}\,\mathrm{d}r, \tag{4.6b}$$

$$\left(r^2 f^{\mathrm{i}}\right)_{j+1/2} = -\int_{r_j}^{r_{j+1}} D^{-1}\mathrm{e}^{-A}\,S\,\mathrm{d}r \Big/ \int_{r_j}^{r_{j+1}} D^{-1}\mathrm{e}^{-A}\,\mathrm{d}r, \tag{4.6c}$$

where $\left(r^2 f^{\mathrm{h}}\right)_{j+1/2}$ and $\left(r^2 f^{\mathrm{i}}\right)_{j+1/2}$ are the homogeneous and inhomogeneous part of $\left(r^2 f\right)_{j+1/2}$, corresponding to the homogeneous and particular solution of (4.1), respectively; cf. (3.3).

To elaborate the expressions in (4.6) we introduce some notation. $\langle a, b\rangle$ denotes the usual inner product of two functions a and b defined on (r_j, r_{j+1}), i.e.,

$$\langle a, b\rangle := \int_{r_j}^{r_{j+1}} a(r)b(r)\,\mathrm{d}r. \tag{4.7}$$

For a generic variable $v > 0$ defined on (r_j, r_{j+1}) we indicate the average, geometric average (of v_j and v_{j+1}) and the harmonic average by $\bar{v}_{j+1/2}$, $\tilde{v}_{j+1/2}$ and $\hat{v}_{j+1/2}$, respectively, i.e.,

$$\begin{aligned} \bar{v}_{j+1/2} &:= \tfrac{1}{2}\left(v_j + v_{j+1}\right), \\ \tilde{v}_{j+1/2} &:= \sqrt{v_j v_{j+1}}, \\ \frac{1}{\hat{v}_{j+1/2}} &:= \frac{\langle v^{-1}, 1\rangle}{\Delta r}. \end{aligned} \tag{4.8}$$

Consider the expression for the homogeneous flux. Assume first that $\varepsilon(r) = \text{Const}$ on (r_j, r_{j+1}). In this case expression (4.6b) can be evaluated as

$$(r^2 f^{\mathrm{h}})_{j+1/2} = \mathcal{F}^{\mathrm{h}}\left(\tilde{D}_{j+1/2}/\Delta r, \tilde{P}_{j+1/2}; \varphi_j, \varphi_{j+1}\right), \quad \tilde{P}_{j+1/2} := \frac{U\Delta r}{\tilde{D}_{j+1/2}}, \tag{4.9}$$

with $\mathcal{F}^{\mathrm{h}}$ defined in (3.6) and $\tilde{P}_{j+1/2}$ the geometric average of P, which we refer to as the constant coefficient homogeneous flux, i.e., $U = r^2 u = \text{Const}$ and $\varepsilon = \text{Const}$. In general,

when ε is an arbitrary function of r, we can derive the following expression

$$\left(r^2 f^{\mathrm{h}}\right)_{j+1/2} = \mathcal{F}^{\mathrm{h}}\left(\hat{D}_{j+1/2}/\Delta r, \langle a, 1\rangle; \varphi_j, \varphi_{j+1}\right). \tag{4.10}$$

In the derivation we used that $D^{-1} = A'/U$ to evaluate the integral in (4.6b). Thus, the flux can be written as the constant coefficient flux (4.9) with $\tilde{D}_{j+1/2}$ and $\tilde{P}_{j+1/2}$ replaced by $\hat{D}_{j+1/2}$ and $\langle a, 1\rangle$, respectively. Note that $\langle a, 1\rangle$ can be interpreted as the average value of the Peclet function P over (r_j, r_{j+1}).

We consider next the expression for the inhomogeneous flux, and first take $\varepsilon(r) = \text{Const}$ on (r_j, r_{j+1}). Substituting the expression for $S(r)$ in (4.6c) and changing the order of integration, we can derive the representation

$$\left(r^2 f^{\mathrm{i}}\right)_{j+1/2} = \Delta r \int_0^1 G(\sigma; \tilde{P}_{j+1/2}, \sigma_{j+1/2})\, r^2(\sigma) s(r(\sigma)) \left(\frac{r(\sigma)}{\tilde{r}_{j+1/2}}\right)^2 \mathrm{d}\sigma, \tag{4.11a}$$

with $\tilde{P}_{j+1/2}$ defined in (4.9) and with G the Green's function for the flux defined in (3.5), provided the normalized coordinate $\sigma(r)$ and the coordinate of the cell boundary $\sigma_{j+1/2}$ are chosen as

$$\sigma(r) = \frac{r - r_j}{\Delta r}\frac{r_{j+1}}{r}, \quad \sigma_{j+1/2} = \sigma(r_{j+1/2}). \tag{4.11b}$$

For arbitrary ε we can generalize (4.11) as follows

$$\left(r^2 f^{\mathrm{i}}\right)_{j+1/2} = \Delta r \int_0^1 G(\sigma; \langle a, 1\rangle, \sigma_{j+1/2})\, r^2(\sigma) s(r(\sigma)) \frac{D(r(\sigma))}{\hat{D}_{j+1/2}} \mathrm{d}\sigma, \tag{4.12a}$$

$$\sigma(r) = \int_{r_j}^{r} a(\eta)\, \mathrm{d}\eta / \langle a, 1\rangle, \tag{4.12b}$$

where the correction factor $D(r(\sigma))/\hat{D}_{j+1/2}$ in (4.12a) is a consequence of the relation $\hat{D}_{j+1/2}\mathrm{d}r = \Delta r\, D(r(\sigma))\mathrm{d}\sigma$. Note that $a(r) > 0$ implies that $\sigma(r)$ defined in (4.12b) is monotonically increasing from 0 to 1 on the interval (r_j, r_{j+1}). Summarizing, the flux $f_{j+1/2}$ is the superposition of the homogeneous and inhomogeneous flux, defined in (4.10) and (4.12), respectively.

To derive expressions for the numerical flux, we need approximations for $\hat{D}_{j+1/2}$, $\langle a, 1\rangle$, and $\sigma_{j+1/2} = \sigma(r_{j+1/2})$ with $\sigma(r)$ defined in (4.12b). Moreover, we need to evaluate the integral in (4.12a). A straightforward evaluation gives $\langle a, 1\rangle = U\Delta r/\hat{D}_{j+1/2}$. To determine the harmonic average $\hat{D}_{j+1/2}$ from (4.8) we replace ε in the integrand by its average $\bar{\varepsilon}_{j+1/2}$ and evaluate the resulting integral exactly. This way we obtain the approximation $\hat{D}_{j+1/2} \approx \bar{\varepsilon}_{j+1/2}\tilde{r}^2_{j+1/2}$. Using the same approximation for ε in the evaluation of the integral in (4.12b) we obtain $\sigma_{j+1/2} = r_{j+1}/(2r_{j+1/2})$. Since $D(r(\sigma))/\hat{D}_{j+1/2} = 1 + \mathcal{O}(\Delta r)$, we omit the term altogether in (4.12a), resulting in an $\mathcal{O}(\Delta r^2)$ error for the inhomogeneous flux. Moreover, since for dominant advection G has a distinct bias toward the upwind end of (r_j, r_{j+1}), we replace

$r^2(\sigma)s(r(\sigma))$ by its upwind value $r_j^2 s_j$. The resulting integral can be evaluated as

$$\int_0^1 G(\sigma; \langle a, 1\rangle, \sigma_{j+1/2})\,\mathrm{d}\sigma = \sigma_{j+1/2} - W(\langle a, 1\rangle).$$

Then, applying all approximations mentioned above, we obtain the numerical flux

$$\left(r^2F\right)_{j+1/2} = \left(r^2F^{\mathrm{h}}\right)_{j+1/2} + \left(r^2F^{\mathrm{i}}\right)_{j+1/2}, \tag{4.13a}$$

$$\left(r^2F^{\mathrm{h}}\right)_{j+1/2} = \mathcal{F}^{\mathrm{h}}\left(D_{j+1/2}/\Delta r, P_{j+1/2}; \varphi_j, \varphi_{j+1}\right), \tag{4.13b}$$

$$\left(r^2F^{\mathrm{i}}\right)_{j+1/2} = \Delta r\left(\sigma_{j+1/2} - W\left(P_{j+1/2}\right)\right) r_j^2 s_j, \tag{4.13c}$$

with coefficients $D_{j+1/2}$, $P_{j+1/2}$ and $\sigma_{j+1/2}$ given by

$$\begin{aligned} D_{j+1/2} &:= \bar{r}_{j+1/2}^2 \bar{\varepsilon}_{j+1/2}, \\ P_{j+1/2} &:= \frac{U\Delta r}{D_{j+1/2}}, \\ \sigma_{j+1/2} &= \frac{r_{j+1}}{2r_{j+1/2}}. \end{aligned} \tag{4.13d}$$

We refer to (4.13) as the complete flux (CF) scheme for spherical coordinates, with as special case the homogeneous flux (HF) scheme (4.13b).

5. Numerical flux for cylindrical coordinates

In this section we present the complete flux scheme for conservation laws in cylindrical coordinates, assuming rotational symmetry about the z-axis. Consequently, the problem does not depend on the azimuthal coordinate θ. We proceed in two steps. First, we derive the r-component of the flux in polar coordinates, so we solve an essentially one-dimensional problem, and second, we extend the scheme by including the z-component, to derive the full two-dimensional scheme.

The stationary, rotationally symmetric conservation law in polar coordinates reads $\mathrm{d}(rf)/\mathrm{d}r = rs$ with $f = u\varphi - \varepsilon \mathrm{d}\varphi/\mathrm{d}r$. We give a very concise derivation of the CF scheme, since it is quite similar to the CF scheme in spherical coordinates. To determine the integral relation for the flux $f_{j+1/2} := f(r_{j+1/2})$, we consider the one-dimensional model BVP:

$$\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\left(u\varphi - \varepsilon\frac{\mathrm{d}\varphi}{\mathrm{d}r}\right)\right) = s, \quad r_j < r < r_{j+1}, \tag{5.1a}$$

$$\varphi(r_j) = \varphi_j, \quad \varphi(r_{j+1}) = \varphi_{j+1}, \tag{5.1b}$$

where ε and s are sufficiently smooth functions of r and where, because of (2.2), u satisfies the relation $U := ru = \text{Const}$. The definitions of the variables a, P and A in (4.3) still hold, whereas the definitions of D and S change to

$$D := \varepsilon r, \quad S(r) := \int_{r_{j+1/2}}^{r} \eta s(\eta)\,\mathrm{d}\eta. \tag{5.2}$$

We can essentially repeat the derivation in the previous section: integrate the conservation law from the cell boundary $r_{j+1/2}$ to $r \in (r_j, r_{j+1})$, rewrite the flux in terms of its integrating factor, substitute the flux in the integral relation and subsequently integrate over the interval (r_j, r_{j+1}), to arrive at the following expressions:

$$\left(rf\right)_{j+1/2} = \left(rf^{\mathrm{h}}\right)_{j+1/2} + \left(rf^{\mathrm{i}}\right)_{j+1/2}, \tag{5.3a}$$

$$\left(rf^{\mathrm{h}}\right)_{j+1/2} = \left(\mathrm{e}^{-A_j}\varphi_j - \mathrm{e}^{-A_{j+1}}\varphi_{j+1}\right) / \int_{r_j}^{r_{j+1}} D^{-1}\mathrm{e}^{-A}\,\mathrm{d}r, \tag{5.3b}$$

$$\left(rf^{\mathrm{i}}\right)_{j+1/2} = -\int_{r_j}^{r_{j+1}} D^{-1}\mathrm{e}^{-A}\,S\,\mathrm{d}r / \int_{r_j}^{r_{j+1}} D^{-1}\mathrm{e}^{-A}\,\mathrm{d}r, \tag{5.3c}$$

thus, as anticipated, the flux $f_{j+1/2}$ is the superposition of the homogeneous flux $f^{\mathrm{h}}_{j+1/2}$ and the inhomogeneous flux $f^{\mathrm{i}}_{j+1/2}$; cf. (4.6).

Next, we have to elaborate (5.3b) and (5.3c). Evaluating all integrals involved, we recover relation (4.10) for the homogeneous flux. Substituting the expression for S in (5.3c) and changing the order of integration, we obtain the expression

$$\left(rf^{\mathrm{i}}\right)_{j+1/2} = \Delta r \int_0^1 G(\sigma; \langle a, 1\rangle, \sigma_{j+1/2})\, r(\sigma) s(r(\sigma))\, \frac{D(r(\sigma))}{\hat{D}_{j+1/2}}\,\mathrm{d}\sigma, \tag{5.4}$$

where the normalized coordinate σ is defined in (4.12b). Finally, to derive expressions for the numerical flux, we need approximations for $\hat{D}_{j+1/2}$, $\langle a, 1\rangle$, $\sigma_{j+1/2}$ and for the integral in the right hand side of (5.4). For the latter, we replace the term $r\,s(r)$ in the integrand by its upwind value $\left(r\,s(r)\right)_{\mathrm{u},j+1/2}$, i.e., $\left(r\,s(r)\right)_{\mathrm{u},j+1/2} = r_j\,s_j$ if $\bar{u}_{j+1/2} \geq 0$ and $\left(r\,s(r)\right)_{\mathrm{u},j+1/2} = r_{j+1}\,s_{j+1}$ if $\bar{u}_{j+1/2} < 0$. Approximating ε by its average $\bar{\varepsilon}_{j+1/2}$, we obtain similar results as in Section 4, except that the harmonic average $\hat{D}_{j+1/2}$ is now approximated as

$$\hat{D}_{j+1/2} \approx \bar{\varepsilon}_{j+1/2}\hat{r}_{j+1/2}, \quad \hat{r}_{j+1/2} = \frac{r_{j+1} - r_j}{\ln\left(r_{j+1}/r_j\right)}.$$

From straightforward Taylor expansions we conclude that $\hat{r}_{j+1/2} = r_{j+1/2} + \mathcal{O}\left(\Delta r^2\right)$. Putting everything together, we obtain the following version of the complete flux scheme:

$$\left(rF\right)_{j+1/2} = \left(rF^{\mathrm{h}}\right)_{j+1/2} + \left(rF^{\mathrm{i}}\right)_{j+1/2}, \tag{5.5a}$$

$$\left(rF^{\mathrm{h}}\right)_{j+1/2} = \mathcal{F}^{\mathrm{h}}\left(D_{j+1/2}/\Delta r, P_{j+1/2}; \varphi_j, \varphi_{j+1}\right), \tag{5.5b}$$

$$\left(rF^{\mathrm{i}}\right)_{j+1/2} = \Delta r\left(\sigma_{j+1/2} - W\left(P_{j+1/2}\right)\right)\left(r\,s\right)_{\mathrm{u},j+1/2}, \tag{5.5c}$$

where the coefficients $D_{j+1/2}$, $P_{j+1/2}$ and $\sigma_{j+1/2}$ are given by

$$D_{j+1/2} := r_{j+1/2}\,\bar{\varepsilon}_{j+1/2}, \quad P_{j+1/2} := \frac{U\Delta r}{D_{j+1/2}}, \quad \sigma_{j+1/2} = \frac{\ln\left(r_{j+1/2}/r_j\right)}{\ln\left(r_{j+1}/r_j\right)}; \tag{5.5d}$$

cf. (4.13). Note that $P_{j+1/2}$ is the average of the Peclet function P over the interval (r_j, r_{j+1}).

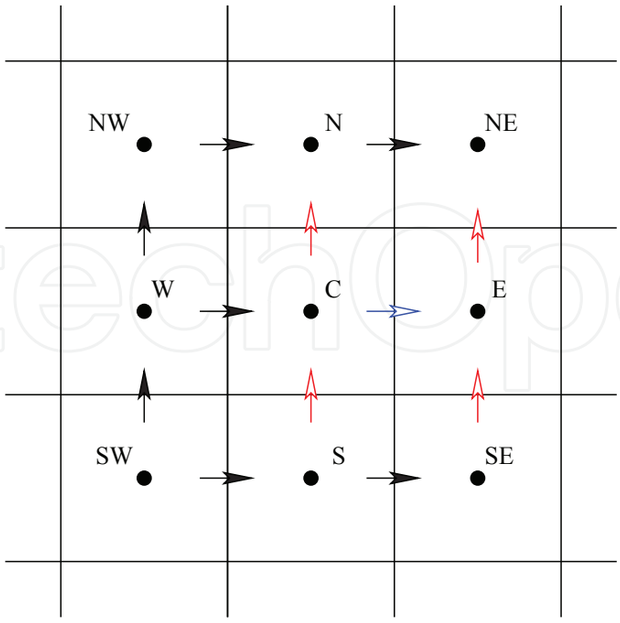

Fig. 3. Control volume Ω_C and corresponding stencil.

Next, we extend the derivation to two-dimensional conservation laws, including the z-component of the flux. In particular, we derive the expression for the r-component of the numerical flux. For ease of notation, we use both index notation and the compass notation; see Figure 3. Thus, φ_C should be undersood as $\varphi_{j,l}$ and $f_{r,e}$ as $f_{r,j+1/2,l}$ etc.

The flux corresponding to equation (2.1) is given by

$$\boldsymbol{f} = f_r \boldsymbol{e}_r + f_z \boldsymbol{e}_z = \Big(u_r \varphi - \varepsilon \frac{\partial \varphi}{\partial r}\Big) \boldsymbol{e}_r + \Big(u_z \varphi - \varepsilon \frac{\partial \varphi}{\partial z}\Big) \boldsymbol{e}_z. \tag{5.6}$$

We outline the derivation of the r-component of the numerical flux $F_{r,j+1/2,l}$ at the eastern edge of the control volume $\Omega_{j,l}$; see Figure 3. The derivation of the z-component $F_{z,j,l+1/2}$ of the numerical flux at the northern edge is completely analogous and is therefore omitted. The key idea is to include the cross flux term $\partial f_z / \partial z$ in the evaluation of the flux. Therefore we determine the numerical flux $F_{r,j+1/2,l}$ from the quasi-one-dimensional BVP:

$$\frac{1}{r} \frac{\partial}{\partial r} \Big(r \Big(u_r \varphi - \varepsilon \frac{\partial \varphi}{\partial r} \Big) \Big) = s_r, \quad r_j < r < r_{j+1}, \, z = z_l, \tag{5.7a}$$

$$\varphi(\boldsymbol{x}_{j,l}) = \varphi_{j,l}, \quad \varphi(\boldsymbol{x}_{j+1,l}) = \varphi_{j+1,l}, \tag{5.7b}$$

where the modified source term s_r is defined by

$$s_r := s - \frac{\partial f_z}{\partial z}. \tag{5.7c}$$

The derivation of the expression for the numerical flux is essentially the same as for (5.5), the main difference being the inclusion of the cross flux term $\partial f_z / \partial z$ in the source term. In the

computation of s_r we replace $\partial f_z/\partial z$ by its central difference approximation and for f_z we take the homogeneous numerical flux. A similar procedure applies to the z-component of the flux, which is actually the Cartesian flux from Section 3, albeit with nonconstant coefficients, [13]. Putting everything together, we obtain the following two-dimensional complete flux scheme.

two-dimensional CF scheme

Peclet function

$$P_r := U_r \Delta r / D \qquad P_z := u_z \Delta z / \varepsilon$$

$$U_r = r u_r, \quad D := r\varepsilon$$

(weighted) average

$$\bar{v}_\mathrm{e} := \tfrac{1}{2}(v_\mathrm{C} + v_\mathrm{E}) \qquad \bar{v}_\mathrm{n} := \tfrac{1}{2}(v_\mathrm{C} + v_\mathrm{N})$$

$$v^*_\mathrm{n} := W(-\bar{P}_{z,\mathrm{n}}) v_\mathrm{C} + W(\bar{P}_{z,\mathrm{n}}) v_\mathrm{N}$$

homogeneous flux

$$\left(rF^\mathrm{h}_r\right)_\mathrm{e} = \mathcal{F}^\mathrm{h}\left(D_\mathrm{e}/\Delta r, P_{r,\mathrm{e}}; \varphi_\mathrm{C}, \varphi_\mathrm{E}\right) \qquad F^\mathrm{h}_{z,\mathrm{n}} = \mathcal{F}^\mathrm{h}\left(\mathcal{E}_\mathrm{n}/\Delta z, \bar{P}_{z,\mathrm{n}}; \varphi_\mathrm{C}, \varphi_\mathrm{N}\right)$$

$$D_\mathrm{e} = r_\mathrm{e}\bar{\varepsilon}_\mathrm{e}, \quad P_{r,\mathrm{e}} = \bar{U}_{r,\mathrm{e}}\Delta r / D_\mathrm{e} \qquad \mathcal{E}_n = P^*_{z,\mathrm{n}}\varepsilon^*_\mathrm{n}/\bar{P}_{z,\mathrm{n}}$$

source term with cross wind diffusion

$$s_{r,\mathrm{C}} = s_\mathrm{C} - \frac{1}{\Delta z}\left(F^\mathrm{h}_{z,\mathrm{n}} - F^\mathrm{h}_{z,\mathrm{s}}\right) \qquad s_{z,\mathrm{C}} = s_\mathrm{C} - \frac{1}{r_\mathrm{C}}\frac{1}{\Delta r}\left(\left(rF^\mathrm{h}_r\right)_\mathrm{e} - \left(rF^\mathrm{h}_r\right)_\mathrm{w}\right)$$

upwinded source term

$$s_{r,\mathrm{u,e}} = \begin{cases} s_{r,\mathrm{C}} & \text{if} \quad \bar{u}_{r,\mathrm{e}} \geq 0 \\ s_{r,\mathrm{E}} & \text{if} \quad \bar{u}_{r,\mathrm{e}} < 0 \end{cases} \qquad s_{z,\mathrm{u,n}} = \begin{cases} s_{z,\mathrm{C}} & \text{if} \quad \bar{u}_{z,\mathrm{n}} \geq 0 \\ s_{z,\mathrm{N}} & \text{if} \quad \bar{u}_{z,\mathrm{n}} < 0 \end{cases}$$

inhomogeneous flux

$$\left(rF^\mathrm{i}_r\right)_\mathrm{e} = \Delta r\left(\sigma_\mathrm{e} - W(P_{r,\mathrm{e}})\right)\left(rs_r\right)_{\mathrm{u,e}} \qquad F^\mathrm{i}_{z,\mathrm{n}} = \Delta z\left(\tfrac{1}{2} - W(\bar{P}_{z,\mathrm{n}})\right) s_{z,\mathrm{u,n}}$$

$$\sigma_\mathrm{e} = \frac{\ln\left(r_\mathrm{e}/r_\mathrm{C}\right)}{\ln\left(r_\mathrm{E}/r_\mathrm{C}\right)}$$

complete flux

$$\left(rF_r\right)_\mathrm{e} = \left(rF^\mathrm{h}_r\right)_\mathrm{e} + \left(rF^\mathrm{i}_r\right)_\mathrm{e} \qquad F_{z,\mathrm{n}} = F^\mathrm{h}_{z,\mathrm{n}} + F^\mathrm{i}_{z,\mathrm{n}}.$$

The stencil of the flux approximation for $F_{r,\mathrm{e}}$ is depicted in Figure 3. Assume first that $\bar{u}_{r,\mathrm{e}} > 0$. Then $F_{r,\mathrm{e}}$ depends on φ in the grid points $\boldsymbol{x}_\mathrm{C}$ and $\boldsymbol{x}_\mathrm{E}$, on s in the central point $\boldsymbol{x}_\mathrm{C}$ and on the homogeneous fluxes $F^\mathrm{h}_{z,\mathrm{n}}$ and $F^\mathrm{h}_{z,\mathrm{s}}$ and through these fluxes again on φ in $\boldsymbol{x}_\mathrm{N}$ and $\boldsymbol{x}_\mathrm{S}$. For $\bar{u}_{r,\mathrm{e}} < 0$, $F_{r,\mathrm{e}}$ again depends on φ_C and φ_E, but this time on the source term s_E and the homogeneous fluxes $F^\mathrm{h}_{z,\mathrm{En}}$ and $F^\mathrm{h}_{z,\mathrm{Es}}$, inducing a further dependency on φ_NS and φ_SE. Thus, in

addition to the direct neighbours, $F_{r,e}$ depends on a few other values of φ, determined by the local upwind direction.

6. Aspects of time integration

Next, we extend the derivation to time-dependent conservation laws, restricting ourselves to spherically symmetric conservation laws; for Cartesian coordinates see [13, 15].

The semidiscrete conservation law for $\varphi_j(t) \approx \varphi(r_j, t)$ can be written as

$$\left(r^2F\right)_{j+1/2}(t) - \left(r^2F\right)_{j-1/2}(t) = \Delta r\left(r_j^2 + \tfrac{1}{12}\Delta r^2\right)\left(s_j(t) - \dot{\varphi}_j(t)\right), \tag{6.1}$$

where $\dot{\varphi}_j(t) \approx \partial\varphi/\partial t(r_j, t)$ and $s_j(t) = s(r_j, t)$. In the following we shall omit the explicit dependence on the variable t.

For the numerical flux $F_{j+1/2}$ in (6.1) we have two options. We can simply take the flux (4.13) derived from the corresponding BVP (4.1), and henceforth referred to as the stationary complete flux (SCF) scheme. Alternatively, we can include $\partial\varphi/\partial t$ in the numerical flux, if we determine $\left(r^2F\right)_{j+1/2}$ from the quasi-stationary BVP:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\left(u\varphi - \varepsilon\frac{\partial\varphi}{\partial r}\right)\right) = s - \frac{\partial\varphi}{\partial t}, \quad r_j < r < r_{j+1}, \tag{6.2a}$$

$$\varphi(r_j) = \varphi_j, \quad \varphi(r_{j+1}) = \varphi_{j+1}, \tag{6.2b}$$

thus subtracting the time derivative from the source term. We can repeat the derivation in Section 4, to arrive at the following expression for the numerical flux

$$\left(r^2F\right)_{j+1/2} = \frac{D_{j+1/2}}{\Delta r}\left(B\left(-P_{j+1/2}\right)\varphi_j - B\left(P_{j+1/2}\right)\varphi_{j+1}\right) + \Delta r\left(\sigma_{j+1/2} - W\left(P_{j+1/2}\right)\right) r_j^2(s_j - \dot{\varphi}_j), \tag{6.3}$$

referred to as the transient complete flux (TCF) scheme; cf. (4.13). This numerical flux can be written in the desired form (2.13) as

$$\left(r^2F\right)_{j+1/2} = \alpha_{j+1/2}\,\varphi_j - \beta_{j+1/2}\,\varphi_{j+1} + \Delta r\left(\gamma_{j+1/2}\,\tilde{s}_j + \delta_{j+1/2}\,\tilde{s}_{j+1}\right), \tag{6.4a}$$

with $\tilde{s} := s - \partial\varphi/\partial t$ and where the coefficient $\alpha_{j+1/2}$ etc. are defined by

$$\begin{aligned}
\alpha_{j+1/2} &:= \frac{D_{j+1/2}}{\Delta r}B^-_{j+1/2},\\
\beta_{j+1/2} &:= \frac{D_{j+1/2}}{\Delta r}B^+_{j+1/2},\\
B^\pm_{j+1/2} &:= B(\pm P_{j+1/2}),\\
\gamma_{j+1/2} &:= \sigma_{j+1/2} - W\left(P_{j+1/2}\right),\\
\delta_{j+1/2} &:= 0.
\end{aligned} \tag{6.4b}$$

A similar expression holds for the numerical flux $F_{j-1/2}$. Substituting the TCF approximations in (6.1) we obtain the finite volume TCF semidiscretisation, given by

$$b_{\mathrm{W},j}\dot{\varphi}_{j-1} + b_{\mathrm{C},j}\dot{\varphi}_j - a_{\mathrm{W},j}\varphi_{j-1} + a_{\mathrm{C},j}\varphi_j - a_{\mathrm{E},j}\varphi_{j+1} = b_{\mathrm{W},j}s_{j-1} + b_{\mathrm{C},j}s_j, \tag{6.5a}$$

where the coefficients $a_{\mathrm{W},j}$ etc. are defined by

$$\begin{aligned} a_{\mathrm{W},j} &:= \alpha_{j-1/2}, \quad a_{\mathrm{E},j} := \beta_{j+1/2}, \quad a_{\mathrm{C},j} := \alpha_{j+1/2} + \beta_{j-1/2}, \\ b_{\mathrm{W},j} &:= \Delta r\,\gamma_{j-1/2}, \quad b_{\mathrm{C},j} := \Delta r\big(r_j^2 + \tfrac{1}{12}\Delta r^2 - \gamma_{j+1/2}\big). \end{aligned} \tag{6.5b}$$

The semidiscretization in (6.5) defines an implicit ODE system, for which we require an A-stable, one-step time integrator. Our choise is the trapezoidal rule. In [15] we have shown that the Cartesian TCF scheme has usually much smaller dissipation and dispersion errors than the corresponding SCF scheme, provided the solution is smooth.

7. Numerical example

In this section we apply the complete flux scheme to a model problem, describing a premixed spherical flame stabilized by a point source of combustible mixture.

A point source at the origin issues a mass flux of $4\pi U$ of combustible mixture. After ignition, a stable spherical flame is formed, provided the value of U is in the proper range. The governing equations for this system are given by [2, 12]:

$$\frac{\partial C}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\Big(UC - r^2\frac{1}{\mathrm{Le}}\frac{\partial C}{\partial r}\Big) = \omega, \quad r > 0, t > 0, \tag{7.1a}$$

$$\frac{\partial T}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\Big(UT - r^2\frac{\partial T}{\partial r}\Big) = \omega, \tag{7.1b}$$

where C and T are the dimensionless concentration of combustion product and temperature, respectively, and where ω is the (dimensionless) reaction rate. The radial coordinate r and the time t are dimensionless as well. Parameters in (7.1) are the mass flux (per solid angle) U and the Lewis number Le. The reaction rate ω depends on C and T as follows

$$\omega = \frac{1}{2\mathrm{Le}}\beta^2(1-Y)\mathrm{e}^{\beta(T-1)}, \tag{7.2}$$

with β the dimensionless activation energy. In the unburnt gas mixture, far ahead of the flame front, there is no combustion product and the temperature equals the temperature of the unburnt gas. In the burnt gas, beyond the flame, we assume that the reaction is completed, and consequently the combustion product is the only species and the temperature is equal to the adiabatic temperature of the burnt gas mixture. These conditions lead to the following boundary conditions

$$C(0,t) = T(0,t) = 0, \quad C(\infty,t) = T(\infty,t) = 1, \quad t > 0. \tag{7.3}$$

As initial conditions, we take the linear profiles $C(r,0) = r/r_{\max}$ and $T(r,0) = r/r_{\max}$ on the truncated domain $(0, r_{\max})$ and let the solution evolve to its steady state. We take $r_{\max} = 120$.

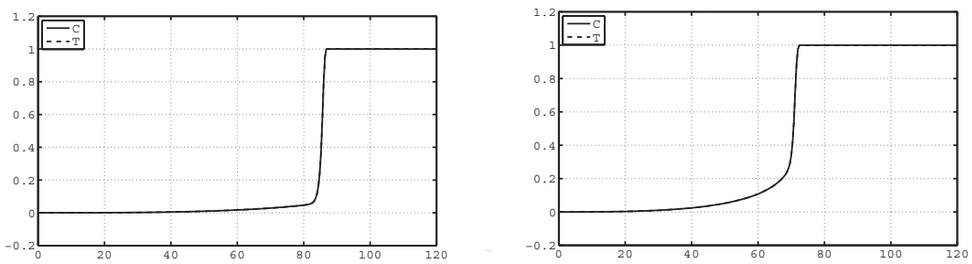

Fig. 4. Numerical solutions of the thermo-diffusive model (7.1) for $\beta = 10$ (left) and $\beta = 8$ (right). Other parameters are: $U = 1.0475 \times 10^4$ and $\mathrm{Le} = 1$.

For space discretisation of (7.1) we employ the TCF scheme (6.4a) in combination with the θ-method for time integration [5]. The resulting nonlinear system at each time step is solved applying one Newton iteration step. Moreover, to enhance the robustness of the method, we bound the numerical solutions according to $0 \leq C_j, T_j \leq 1$, followed by a smoothing step as follows: $C_j := \frac{1}{4}\left(C_{j-1} + 2C_j + C_{j+1}\right)$, and likewise for T_j.

As an example, the numerical solutions at $t = 100$ for $U = 1.0475 \times 10^4$, $\mathrm{Le} = 1$ and $\beta = 10, 8$ are shown in Figure 4, computed with grid size $\Delta r = 0.4$ and time step $\Delta t = 0.25$. The solutions exhibit a steep interior layer, the so-called flame front, connecting the (virtually) constant unburnt and burnt states. Since $\mathrm{Le} = 1$, the numerical solutions for C and T are identical. The solution for $\beta = 10$ is very close to the asymptotic solution [12]

$$C(r,0) = \begin{cases} \exp\left(\mathrm{Le}U\left(\frac{1}{r_\mathrm{f}} - \frac{1}{r}\right)\right) & \text{if} \quad r \leq r_\mathrm{f}, \\ 1 & \text{if} \quad r \geq r_\mathrm{f} \end{cases},$$

$$T(r,0) = \begin{cases} \exp\left(U\left(\frac{1}{r_\mathrm{f}} - \frac{1}{r}\right)\right) & \text{if} \quad r \leq r_\mathrm{f}, \\ 1 & \text{if} \quad r \geq r_\mathrm{f}, \end{cases},$$

with $r_\mathrm{f} = 93.4$ the radius of the flame. For decreasing β the reaction slows down, resulting in a slightly wider flame front and a location of the flame front closer to the source. We define $e_C := \left|\left|\left(\boldsymbol{C}^{n+1} - \boldsymbol{C}^n\right)/\Delta t\right|\right|_1 / N$ with $\boldsymbol{C}^n = \left(C_j^n\right)^\mathrm{T}$ and N the number of grid points, and likewise e_T. The time histories of e_C and e_T corresponding to the numerical solutions in Figure 4 are shown in Figure 5. We observe a regular convergence to the steady state. Finally, in order to study the effect of preferential diffusion, the numerical simulations are repeated for $\mathrm{Le} = 0.3$, and the results are shown in Figure 6. As expected, the interior layer for C is slightly wider than for T.

8. Conclusions and future research

In this paper we have derived complete flux schemes for spherically or cylindrically symmetric conservation laws of advection-diffusion-reaction type. An integral relation for the flux is derived from a local one-dimensional BVP for the *entire* equation, including

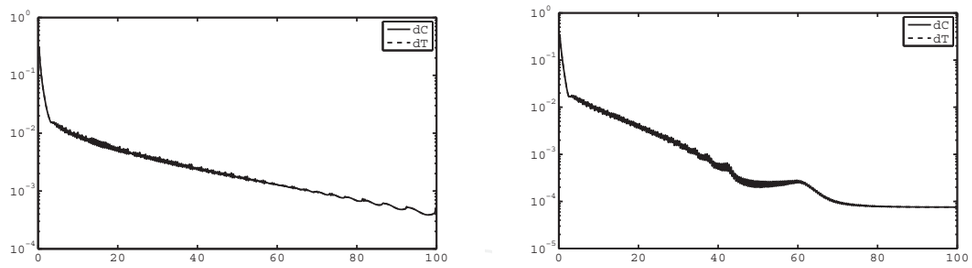

Fig. 5. Time history of the (discrete) time derivatives. Parameter values are: $\beta = 10$ (left), $\beta = 8$ (right), $U = 1.0475^4$ and $\mathrm{Le} = 1$.

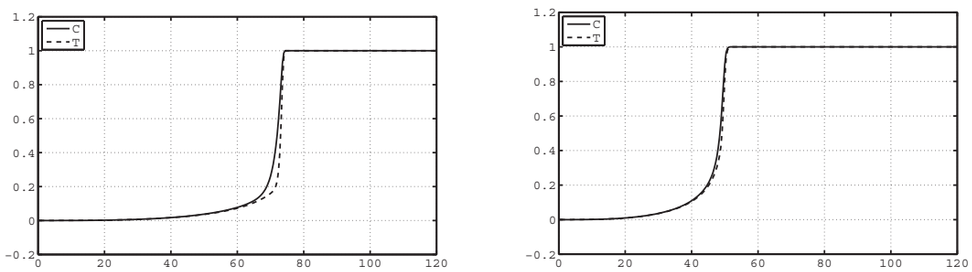

Fig. 6. Numerical solutions of the thermo-diffusive model (7.1) for $\beta = 10$ (left) and $\beta = 8$ (right). Other parameters are: $U = 1.0475 \times 10^4$ and $\mathrm{Le} = 0.3$.

the source term. Applying suitable quadrature rules, we derived expressions for the numerical flux. As a result of this procedure, we obtained a numerical flux that is the superposition of a homogeneous flux, corresponding to the advection-diffusion operator, and an inhomogeneous flux, corresponding to the reaction term. For time-dependent conservation laws, we included the time derivative in the inhomogeneous flux, resulting in an implicit ODE system. The CF-scheme has been applied to a thermo-diffusive model for a spherical flame.

Possible directions of future research are the following: first, a rigourous convergence analysis of the (stationary) CF-schemes for spherical and cylindrical coordinates, and second, a dispersion analysis of time-dependent CF scheme; cf. [15] where such analysis is presented for Cartesian coordinates. Finally, from a more fundamental point of view, it would be very interesting to base the derivation of the time-dependent CF scheme on a local initial-boundary-value problem for a truly time-dependent equation, rather than computing the flux from a quasi-stationary BVP.

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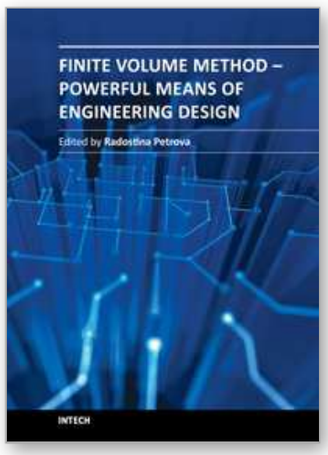

Finite Volume Method - Powerful Means of Engineering Design
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