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Numerical Solution of Reservoir Flow Models based on
large Time Step Operator splitting Algorithms

by

Magne S. Espedal and Kenneth H. Karlsen

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NUMERICAL SOLUTION OF RESERVOIR FLOW MODELS BASED ON LARGE TIME STEP OPERATOR SPLITTING ALGORITHMS

— C.I.M.E. LECTURE NOTES —

MAGNE S. ESPEDAL AND KENNETH HVISTENDAHL KARLSEN

ABSTRACT. During recent years the authors and collaborators have been involved in an activity related to the construction and analysis of large time step operator splitting algorithms for the numerical simulation of multi-phase flow in heterogeneous porous media. The purpose of these lecture notes is to review some of this activity. We illustrate the main ideas behind these novel operator splitting algorithms for a basic two-phase flow model. Special focus is posed on the numerical solution algorithms for the saturation equation, which is a convection dominated, degenerate convection-diffusion equation. Both theory and applications are discussed. The general background for the reservoir flow model is reviewed, and the main features of the numerical algorithms are presented. The basic mathematical results supporting the numerical algorithms are also given. In addition, we present some results from the *BV* solution theory for quasilinear degenerate parabolic equations, which provides the correct mathematical framework in which to analyse our numerical algorithms. Two- and three-dimensional numerical test cases are presented and discussed. The main conclusion drawn from the numerical experiments is that the operator splitting algorithms indeed exhibit the property of resolving accurately internal layers with steep gradients, give very little numerical diffusion, and, at the same time, permit the use of large time steps. In addition, these algorithms seem to capture all potential combinations of convection and diffusion forces, ranging from convection dominated problems (including the pure hyperbolic case) to more diffusion dominated problems.

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1. INTRODUCTION

The flow in subsurface hydrology and the exploitation of hydrocarbons in a reservoir represent very complex processes of controlling the interaction between several fluids and the rock [43, 69, 111]. Capillary and gravity forces are important for the dynamics, and the presence of heterogeneities in natural formations have a large effect on the flow. Accurate modelling of the rock lithology, including the modelling of scale dependent physical parameters and relations, is crucial for obtaining reliable results. The dynamics of the porous media itself add to the complexity. Change in the pressure balance between the overburden pressure and the fluid pressure in the reservoir will change porosity and permeability. Temperature gradients created by injecting fluids having lower temperature than the reservoir will create cracking which can effect the flow properties strongly. Models for flow dynamics should therefore be coupled to a geodynamical model

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describing the dynamics of the rock. Often a reservoir has horizontal wells with several branches, and the coupling between the wells and the reservoir represents a very difficult modelling task.

A series of models [8, 35, 121] have been constructed to describe the complex dynamics of reservoir flow processes. A black-oil model is commonly used to describe water injection. This model works well in simulating water flooding processes because reservoir hydrocarbons are not soluble in the water phase. But it may not be well suited when the composition of the reservoir fluid is dramatically changed because of chemical reactions. Consequently, fluid properties and phase behaviour should in many cases be functions of reservoir pressure, temperature, and fluid composition. The geological model together with the chemical and physical complexity of multi-phase, multi-component flow pose very large and difficult problems to solve. However, the vast expansion of computational capability has made a quantitative description of more realistic and complex models possible. Along with this development, there has also been a very active development of new numerical solution algorithms for such models.

The fluid flow models usually represent strongly coupled systems of nonlinear partial differential equations. A number of new algorithms [79, 90, 105, 113, 122, 135, 146] for the solution of (systems of) nonlinear partial differential equations have been developed over the years. But still there is acute need for better solution algorithms as well as mathematical theory supporting them (and the models). The different scales of variation appearing in a reservoir flow model demand an adaptive adjustment of the solution algorithm to the problem at hand. For compressible fluid or rock models, numerical algorithms which provide local conservation properties are needed. Moreover, the transport part of these models needs accurate pressure and velocity calculations. To resolve these issues one may need efficient finite volume methods, see, e.g., [1, 2, 3].

There is a close relationship between the challenges in mathematical and numerical modelling and the development of mathematical and numerical tools. An example is provided by operator splitting algorithms which calculate an approximate transport in a first step. These algorithms have become an important part of many solution methods for fluid dynamics, see, e.g., [11, 78, 101, 128, 144], and reservoir dynamics, see, e.g., [58, 94, 156]. The main purpose of these lecture notes is to present some recently developed operator splitting algorithms for models describing reservoir flow [8, 35, 121] and certain sedimentation processes [23, 25, 38], as well as other models that can be reduced to a sequence of nonlinear convection-diffusion equations.

The reservoir flow model considered in these notes contains a flow equation which is a highly nonlinear parabolic partial differential equation with a strong transport term. One important characteristic of the model is the degeneracy of the second order diffusion operator in the flow equation. The diffusion operator may be zero pointwise, it can be small or zero in regions of the solution space, and fairly large for other values of the solution. Consequently, solutions of the flow equation will in general possess minimal smoothness. The correct mathematical framework in which to treat such nonlinear partial differential equations — as well as to analyse their numerical solution algorithms — is provided by the *BV* solution theory (analysis in classes of discontinuous functions) [151]. For completeness, we will recall some important results from the *BV* solution theory for second order partial differential equations. Mathematical theory supporting the numerical algorithms have been developed within the *BV* solution framework, and central elements of this theory will be presented in a simplified context.

Roughly speaking, one may say that the splitting algorithms simplify the original problem into a hyperbolic problem and an almost symmetric (degenerate) parabolic problem, each of which is solved separately by suitable numerical methods. The main feature of the operator splitting algorithms is the ability to use long time steps and, at the same time, keep the numerical diffusion at a minimum. Several numerical examples will be given to illustrate these and other properties of the splitting algorithms. The nonlinearity inherent in the models gives a rich variation in the solutions. In particular, the solutions may develop sharp or even discontinuous fronts that propagate throughout the reservoir. Also, fractured and faulted regions may create large variations in the solutions. Local grid refinement techniques may therefore be necessary in order to resolve the physical phenomena within the limits of a computational model. Combining operator splitting and domain decomposition algorithms, we get very flexible adaptive mesh refinement and coarsening techniques [47, 129].

The remaining part of these notes is organised as follows: In §2, we present and discuss the reservoir flow model. This basic model consists of an elliptic equation which is coupled to a nonlinear convection-diffusion equation. A sequential time marching strategy will be used to decouple the equations. Since the solution algorithm for the elliptic equation is well described in the literature, we focus in these lecture notes entirely on the convection-diffusion equation. In §3, we recall a few results from the *BV* solution theory for first and second order nonlinear partial differential equations. In §4, we give a fairly thorough presentation of the novel operator splitting algorithms for nonlinear convection-diffusion equations. Both analytical and numerical results for the splitting algorithms are presented. In §5, two numerical methods for hyperbolic problems are presented. In §6, numerical methods for parabolic problems are presented. Finally, two reservoir simulation examples are presented and discussed in §7.

2. THE RESERVOIR FLOW MODEL

A reservoir may consist of several different types of sediments, which in general have different porosity, absolute permeability, relative permeabilities, and capillary pressure. To efficiently compute the solution of the nonlinear system of reservoir flow equations, one should carefully choose the primary variables based on all aspects of the computations and the inherent physics [8]. The pressure gradient is the driving force that causes the flow of reservoir fluids. Thus pressure should be chosen as a primary variable to describe the flow process. Normally a pressure equation is obtained by making a summation over all components and phases in the model. Below we give a pressure equation for a two-component, two-phase model which is derived in this way. For compressible flow, a mass balance formulation of the pressure equation based on a finite volume discretization is a better choice, see Reme et al. [130, 131]. Since the temperature T can vary, it should also be chosen as a primary variable. The temperature is normally governed by a convection-diffusion equation, see [130, 131]. Moreover, $N + 1$ primary variables are needed to characterise the component-transport phenomena (one water component and N hydrocarbon components). If the moles of component i in phase j (for $i = w, 1, \dots, N$ and $j = w, o, g$), which we denote by m_j^i , is chosen as the primary variable for the i th component, the component-transport equations become coupled with strongly nonlinear phase equilibrium constraints. Consequently, computing the solution of the overall system can be extremely expensive. Furthermore, m_j^i is less smooth than the total moles of the component, i.e.,

$$(1) \quad m^i = \sum_{j=o,g,w} m_j^i.$$

Thus a numerical approximation of m^i will be more accurate than an approximation of m_j^i , which also affects the accuracy of the overall approximations. Based on these observations, we choose m^i as the primary variable for the i th component. In this way the solution of the component-transport equations is decoupled from the computation of the phase equilibrium, which in turn reduces the nonlinearity inherent in the reservoir flow model. Since mass is exchanged between phases, component mass is not conserved within each phase, but the total mass of each component is conserved. The corresponding mass conservation can be described by the system of equations

$$(2) \quad \partial_t(\phi m^i) + \nabla \cdot \left(\sum_{j=o,g,w} c_j^i \xi^i v_j + d \nabla m^i \right) = q^i, \quad i = w, 1, \dots, N,$$

where m^i is defined in (1), ϕ is the porosity of the rock, q^i is the molar flow rate of component i , c_j^i is the mole fraction of component i in phase j , ξ^i is the molar density of component i , d represents diffusion, and the Darcy velocities are given as

$$(3) \quad v_j = -\lambda_j(s_j)K(x)(\nabla p_j - \rho_j g \nabla h), \quad j = w, o, g.$$

In (3), h is the height, g is the gravity constant, and ρ_j is the density of phase j . Furthermore, $K(x)$ is the absolute permeability of the rock, which may be a full tensor for anisotropic and heterogeneous porous media, $k_{rj}(s_j)$ are the relative permeabilities, μ_j are the viscosities of the fluids, s_j is the saturation of phase j , $\lambda_j = k_{rj}/\mu_j$ are the phase mobilities. In addition, the nonlinear partial differential equations presented above are coupled with a complex phase package

that describes the relative phase equilibrium for a given pressure-volume-temperature through the equation of state (e.g., the Peng-Robinson equation of state). The phase saturations s_j , mole fractions c_i^j , and other secondary variables are determined by the thermodynamic equations. The fluid dynamics in a porous media may be influenced by changes in the properties of the rock. This means that we must also couple the flow model to a geomechanical model.

The molar mass model presented above gives a nonlinear system of convection-diffusion equations. We will in these notes use a two-component, two-phase, immiscible flow model as our main test case. This simplified model contains many of the mathematical and numerical challenges present in the general model described above. For the two-phase model, (2) can be expressed in terms of the phase saturations. Let $s = s_w$ denote the water saturation (and $1 - s$ the oil saturation). Then the incompressible displacement of oil by water in a porous medium can be described by the following set of partial differential equations (given in dimensionless form):

$$(4) \quad \nabla \cdot v = q_1(x),$$

$$(5) \quad v = -K(x)\lambda(x, s)(\nabla p - \rho(s)\nabla h),$$

$$(6) \quad \phi(x)\partial_t s + \nabla \cdot (f(s)v + f_g(s)K\nabla h) - \varepsilon\nabla \cdot (d(x, s)\nabla s) = q_2(x),$$

where q_1 and q_2 denote the injection/production wells, ε is a dimensionless scaling parameter, $v = v_w + v_o$ is the total Darcy velocity, $\lambda(x, s)$ denotes the total mobility of the phases,

$$\lambda(x, s) = \lambda_w(x, s) + \lambda_o(x, s).$$

We assume that the immobile water and oil are the same in different types of sediments, so that the saturation can be normalised globally. Furthermore, since the mobility is assumed to be constant in each sediment, we will from now on drop the space dependence in λ and λ_j . In (5), p is the global pressure [35]

$$(7) \quad p = \frac{1}{2}(p_w + p_o) + \frac{1}{2} \int_{s_c}^s \left(\frac{\lambda_o - \lambda_w}{\lambda} \frac{\partial p_c}{\partial \xi} \right) d\xi,$$

where p_w and p_o denotes the pressure of water and oil, respectively, $p_c(x, \xi)$ ($= p_o - p_w$) is the capillary pressure function (see (11) below), s_c is chosen such that $p_c(x, s_c) = 0$. In equations (5)-(6), we have

$$\rho(s) = g(\lambda_w \rho_w + \lambda_o \rho_o),$$

and

$$f_g(s) = (\rho_w - \rho_o)f(s)\lambda_o.$$

Equation (6) is the fractional flow formulation of the mass balance equation for water. The fractional flow function $f(s)$, which is typically an S-shaped function of s , is given as

$$(8) \quad f(s) = \frac{\lambda_w(s)}{\lambda_w(s) + \lambda_o(s)}.$$

The diffusion function is given as

$$(9) \quad d(x, s) = -K(x)f(s)\lambda_o(s)\frac{\partial p_c}{\partial s},$$

where the derivative of the capillary pressure function $p_c(x, s)$ is assumed to be negative, see (11) below. We refer to [8, 35, 121] (see also [6]) for a complete survey and justification of the model.

For computational purposes, the analytical forms for the relative permeabilities are chosen as

$$(10) \quad k_{rw} = s^p, \quad k_{ro} = (1 - s)^q, \quad p, q = 2 \text{ or } 3.$$

The capillary pressure may depend on the porosity and the permeability of the rock. We use a capillary pressure function of the form [57]

$$(11) \quad p_c(x, s) = 0.9 \cdot \phi^{-0.9} K^{-\beta} \frac{1-s}{\sqrt{s}}, \quad \beta > 0.$$

Note that the form of (10) and (11) imply that the global pressure function (7) is well-defined. In Figure 1 a), the variation of the convection term in the saturation equation (6) is shown for different values of the gravity term with a constant Darcy velocity v . In Figure 1 b), the diffusion function is plotted for different permeabilities. Note that the diffusion function (9) vanishes for $s = 0, 1$, and that it can be very small in regions close to these endpoints, see Figure 1 b). This means that (6) is a degenerate parabolic equation and close to being strongly degenerate in regions of the solution space. Mathematical and numerical theory for (strongly) degenerate parabolic equations will be given in §3 and §6.1, respectively.

The reservoir flow equations (4)-(5)-(6) are nonlinearly coupled. A sequential time marching strategy will be used to decouple the equations, see §7 for details. The pressure-velocity equations (4)-(5) are solved in a first step using standard finite element and domain decomposition methods, which are well documented in the literature [7, 138, 140]. We will in these lecture notes therefore limit our presentation to solution algorithms for the convection-diffusion equation (6).

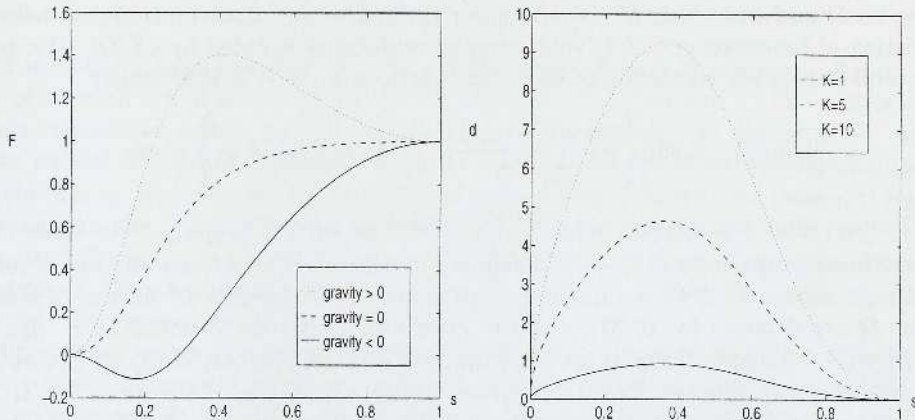


FIGURE 1. a). $F(x, s) = f(s)v + f_g(s)K\nabla h$ plotted as a function of saturation for a fixed Darcy velocity $v = 1$, permeability $K = 1$, and ∇h equal to $-1, 0$, and 1 . b). $d(x, s)$ plotted as a function of saturation for $\beta = 0.1$ and permeabilities K equal to $1, 5$, and 10 .

3. BASIC MATHEMATICAL THEORY

The main purpose of this section is to recall some results from the theory of BV solutions for second order nonlinear (or more precisely quasilinear) partial differential equations. For completeness, we also recall a few basic results from the theory of entropy solutions for hyperbolic partial differential equations. Although the main portion of our work is related to the design of numerical algorithms for the saturation equation (6), the mathematical theory presented below has been important for both the development and the analysis of these algorithms. We have tried to make this section (relatively) self-contained. Nevertheless, it presupposes that the reader has some basic knowledge about functional analysis, measure theory and BV theory, and thus no attempts have been made to discuss in detail the various function spaces, (semi) norms and compactness theories that are used in these lecture notes. The reader who is primarily interested in numerical solution algorithms can skip this section.

We do not claim completeness or technical generality. In fact, a significant limitation of our presentation is that only the Cauchy problem for homogeneous partial differential equations without a source term is discussed. But we stress that the L^1/BV solution theory outlined below also applies (with necessary modifications) to various boundary value problems as well as partial differential equations with variable coefficients and a source term.

Numerical algorithms and the techniques used for their analysis tend to be very different in the two limiting cases of hyperbolic and parabolic equations, see, e.g., [122]. However, independently of whether the problem is hyperbolic or parabolic, in this work *all* the analysis is carried out within

the framework provided by the BV solution theory. Since we try to approximate solutions which in general possess minimal smoothness (due to hyperbolic dominance and parabolic degeneracy), the BV framework is well suited for our purpose. Moreover, the BV framework is also consistent with the theory of entropy solutions for hyperbolic partial differential equations.

Later we show that our numerical approximations converge to the solution of the underlying problem as the discretization parameters tend to zero (see §4). The convergence proof is based on deriving uniform L^∞ and BV (space) estimates for the numerical approximations. These two estimates are then used to show that the approximations are uniformly L^1 continuous in time, and therefore compact in L^1_{loc} . Compactness arguments are classical in the context of hyperbolic partial differential equations and go back to Oleĭnik [124]. The advantage of this “hyperbolic approach” is that the derived estimates are independent of the lower bound on the diffusion coefficient. Consequently, the convergence results are also valid in the degenerate parabolic case.

If Ω is a domain in \mathbb{R}^n , $n \geq 1$, then $C^p(\Omega)$, $p = 1, \dots, \infty$, denotes the space of functions $z : \Omega \rightarrow \mathbb{R}$ possessing continuous partial derivatives of order $\leq p$. When there is no ambiguity, we omit the set Ω and write only C^p (similarly for the spaces and norms introduced below). The space consisting of functions in $C^p(\Omega)$ with compact support is denoted by $C^p_0(\Omega)$. We denote by $Lip(\Omega)$ the Lipschitz space consisting of bounded functions $z : \Omega \rightarrow \mathbb{R}$ that satisfy

$$(12) \quad \|z\|_{Lip(\Omega)} = \sup \left\{ \left| \frac{z(y_2) - z(y_1)}{y_2 - y_1} \right| : y_1, y_2 \in \Omega, y_1 \neq y_2 \right\} < \infty.$$

If $\left| \frac{z(y_2) - z(y_1)}{y_2 - y_1} \right|$ in (12) is replaced by $\max(0, \frac{z(y_2) - z(y_1)}{y_2 - y_1})$, we write $\|z\|_{Lip^+(\Omega)}$. The space of locally Lipschitz continuous functions $z : \Omega \rightarrow \mathbb{R}$ is denoted by $Lip_{loc}(\Omega)$, i.e., functions whose restriction to any compact subset $\mathcal{K} \subset \Omega$ is Lipschitz continuous. The classical L^p spaces of real-valued functions on Ω are denoted by $L^p(\Omega)$, and the norms on $L^p(\Omega)$ are denoted by $\|\cdot\|_{L^p(\Omega)}$. We denote by $L^p_{loc}(\Omega)$ the space of functions on Ω that are in $L^p(\mathcal{K})$ for any compact subset $\mathcal{K} \subset \Omega$.

As we have tried to indicate above, the space $BV(\Omega)$ consisting of functions $z : \Omega \rightarrow \mathbb{R}$ of bounded variation is of fundamental importance to us. A function $z \in L^1_{loc}(\Omega)$ is an element of $BV(\Omega)$ if and only if its first order distributional derivatives are represented by locally finite Borel measures on Ω , i.e., if there exist Borel measures μ_j , $j = 1, \dots, n$, such that

$$-\int_{\Omega} z \frac{\partial \phi}{\partial y_j} dy = \int_{\Omega} \phi d\mu_j, \quad \forall \phi \in C_0^\infty(\Omega),$$

and

$$|\mu_j|(\mathcal{K}) < \infty \text{ for each compact subset } \mathcal{K} \subset \Omega,$$

where $|\mu_j|$ denotes the total variation of the measure μ_j . Let the total variation of $z \in L^1_{loc}(\Omega)$, which we denote by $|z|_{BV(\Omega)}$, be defined as

$$|z|_{BV(\Omega)} = \sup \left\{ \int_{\Omega} z \nabla \cdot \phi dy : \phi \in C_0^\infty(\Omega; \mathbb{R}^n), |\phi(y)| \leq 1, \forall y \in \Omega \right\}.$$

Then using Riesz's theorem on functionals in the space of continuous functions, we obtain that $BV(\Omega)$ can be equivalently defined as

$$BV(\Omega) = \left\{ z \in L^1_{loc}(\Omega) : |z|_{BV(\Omega)} < \infty \right\}.$$

We say that $z(y)$ has bounded Tonelli variation if for any $j = 1, \dots, n$, $u(y)$ considered as a function of y_j has essential (up to the set of one-dimensional measure zero) variation which is integrable with respect to the other variables $y_1, \dots, y_{j-1}, y_{j+1}, \dots, y_n$. A function $z(y)$ is in $BV(\Omega)$ if and only if the Tonelli variation of $z(y)$ is bounded. Furthermore, $z \in BV(\Omega)$ if and only if there is a constant C such that for any $h \in \mathbb{R}^n$ with $y + h \in \Omega$,

$$\int |z(y+h) - z(y)| dy \leq C|h|.$$

The space $BV(\Omega)$ is a Banach space when equipped with the norm

$$\|z\|_{BV(\Omega)} = \|z\|_{L^1(\Omega)} + |z|_{BV(\Omega)}.$$

It is well known that the following inclusions hold:

$$BV(\Omega) \subset L^{\frac{n}{n-1}}(\Omega) \text{ for } n > 1 \text{ and } BV(\Omega) \subset L^\infty(\Omega) \text{ for } n = 1.$$

Furthermore,

$$BV(\Omega) \text{ is compactly imbedded into } L^p(\Omega) \text{ for } 1 \leq p < \frac{n}{n-1}.$$

After a possible modification of $z(y)$ on a set of zero n -dimensional Lebesgue measure, the domain Ω of definition of $z(y)$ is the disjoint union of a set A_z of points of approximate continuity, a set Γ_z of points of approximate jump discontinuity, and a set I_z of irregular points:

$$\Omega = A_z \cup \Gamma_z \cup I_z.$$

The set of irregular points has zero $(n-1)$ -dimensional Hausdorff measure. Hence, with the exception of a small set of irregular points, an arbitrary BV function $z : \Omega \rightarrow \mathbb{R}$ is either approximately continuous or has an approximate jump discontinuity. If $z(y)$ is a BV solution of a nonlinear partial differential equation, the set Γ_z can be thought of as representing the discontinuities (shocks) in $z(y)$, the set A_z as representing the discontinuity free (smooth) region, and I_z as representing the points of shock formation and shock collision. We refer to [55] (and the references cited therein) for a more complete discussion and interpretation of the sets A_z, Γ_z, I_z in the context of BV solutions of hyperbolic partial differential equations. For an introduction to BV (solution) theory, we refer to [61, 148, 149, 151, 167].

For completeness, we recall a few results from the Kruřkov theory of entropy solutions for scalar hyperbolic partial differential equations. For an introduction to general theory for hyperbolic problems, we refer to [90, 120, 141]. We consider nonlinear hyperbolic problems of the form

$$(13) \quad \begin{cases} \partial_t u + \nabla \cdot f(u) = 0, & (x, t) \in \Pi_T = \mathbb{R}^m \times (0, T), \quad m \geq 1, \\ u(x, 0) = u_0(x), & x \in \mathbb{R}^m, \end{cases}$$

where $u : \Pi_T \rightarrow \mathbb{R}$ is the unknown function. We always assume that the vector valued flux function $f = (f_1, \dots, f_m)$ is sufficiently smooth (e.g., in Lip_{loc}) and that the initial function u_0 belongs to $L^1 \cap L^\infty \cap BV$. It is well known that nonlinearity has dramatic effects on hyperbolic waves, most notably in the formation of shock waves (discontinuous solutions), a feature that can reflect the physical phenomenon of breaking of waves. Due to this loss of regularity it is necessary to work with weak solutions. For hyperbolic equations, due to neglected physical (e.g., dissipative) mechanisms, weak solutions are not uniquely determined by their initial data. However, weak solutions satisfying an entropy condition (see below) are uniquely determined by their data.

Recall that a weak solution of the Cauchy problem (13) is a bounded measurable function $u(x, t)$ that satisfies the integral identity

$$(14) \quad \iint \left(u \partial_t \phi + f(u) \cdot \nabla \phi \right) dt dx + \int u_0(x) \phi(x, 0) dx = 0,$$

for all test functions $\phi \in C_0^\infty(\Pi_T)$ such that $\phi|_{t=T} = 0$. Let $\eta : \mathbb{R} \rightarrow \mathbb{R}$ be a convex C^2 function, often referred to as the entropy function, and q_1, \dots, q_m the associated entropy fluxes satisfying the compatibility conditions

$$(15) \quad q'_j(u) = \eta'(u) f'_j(u), \quad j = 1, \dots, m.$$

We let q denote the vector (q_1, \dots, q_m) . Let u denote the L^1_{loc} limit of classical solutions u_ε of the parabolic regularization

$$(16) \quad \partial_t u_\varepsilon + \nabla \cdot f(u_\varepsilon) = \varepsilon \Delta u_\varepsilon, \quad u_\varepsilon(x, 0) = u_0(x),$$

as $\varepsilon \rightarrow 0$. Equipped with the compatibility conditions (15), it is straightforward to show that the "vanishing viscosity" limit u satisfies the entropy inequality

$$\iint \left(\eta(u) \partial_t \phi + q(u) \cdot \nabla \phi \right) dt dx \geq 0,$$

for all non-negative $\phi \in C_0^\infty(\Pi_T)$, see Kruřkov [108]. By a limiting argument, we can let

$$\eta(u) \rightarrow |u - k|,$$

for any given $k \in \mathbb{R}$, and use

$$q(u) = \text{sign}(u - k)(f(u) - f(k)).$$

We thus end up with the following definition due to Kruřkov [108] (see also Vol'pert [148]):

Definition 3.1. *A weak solution $u(x, t)$ of (13) is called an entropy weak solution if, for all non-negative test functions $\phi \in C_0^\infty(\Pi_T)$ and $k \in \mathbb{R}$,*

$$(17) \quad \iint \left(|u - k| \partial_t \phi + \text{sign}(u - k)(f(u) - f(k)) \cdot \nabla \phi \right) dt dx \geq 0.$$

Kruřkov [108] (see also [13, 109]) proved that an entropy weak solution of (13) is uniquely determined by its initial data, and thus coincides with the vanishing viscosity solution. More precisely, he proved the following result: If u and v are entropy weak solutions of (13) with initial data u_0 and v_0 , respectively, then

$$(18) \quad \|u(\cdot, t) - v(\cdot, t)\|_{L^1} \leq \|u_0 - v_0\|_{L^1}.$$

We note that Vol'pert [148] only proved uniqueness of entropy weak solutions in the BV class. We also note that the Kruřkov theory for the pure initial value problem (13) can be extended to the initial-boundary value problem, see Bardos, LeRoux, and Nédélec [9] and Otto [126] for details.

Soon after the penetrating work of Kruřkov, it was realized by Kuznetsov [110] that the method of "doubling of the variables" could be used to establish a general approximation theory for entropy solutions of hyperbolic partial differential equations. In the subsequent years, the theory of Kuznetsov was used (by himself and others) to derive error estimates for the method of vanishing viscosity as well as many numerical methods. We refer to [90] for an introduction to this theory. For recent contributions to the approximation theory of entropy solutions, we refer to Cockburn and Gremaud [36], Bouchout and Perthame [18], Perthame [127], and Tadmor [142].

For completeness, we recall that the solution of (13) satisfies following estimates:

Theorem 3.1. *Let u, v be entropy weak solutions of the hyperbolic problems*

$$\begin{aligned} \partial_t u + \nabla \cdot f(u) &= 0, & u|_{t=0} &= u_0, \\ \partial_t v + \nabla \cdot g(v) &= 0, & v|_{t=0} &= v_0. \end{aligned}$$

Then we have

$$(19) \quad \|u(\cdot, T) - v(\cdot, T)\|_{L^1} \leq \|u_0 - v_0\|_{L^1} + T \min(|u_0|_{BV}, |v_0|_{BV}) \max_j \|f_j - g_j\|_{\text{Lip}}.$$

Furthermore, the unique entropy weak solution of (13) satisfies the following estimates:

$$(20) \quad \begin{cases} \text{(a)} & \|u(\cdot, t)\|_{L^\infty} \leq \|u_0\|_{L^\infty}, \\ \text{(b)} & |u(\cdot, t)|_{BV} \leq |u_0|_{BV}, \\ \text{(c)} & \|u(\cdot, t_2) - u(\cdot, t_1)\|_{L^1} \leq \text{Const} \cdot |t_2 - t_1|, \quad \forall t_1, t_2 \geq 0. \end{cases}$$

The first part of this theorem was first proved by Lucier [119] in the one-dimensional case, and in [93] and by Bouchut and Perthame [18] in the multi-dimensional case. It can also be obtained by using Theorem 3.3 below and then passing to the limit in the parabolic regularization (16). The second part of the theorem follows, e.g., from the estimates derived by Kruřkov [108].

For later use, let us recall a few additional facts about entropy weak solutions of the one-dimensional conservation law

$$(21) \quad \begin{cases} \partial_t u + \partial_x f(u) = 0, & (x, t) \in \mathbb{R} \times (0, T), \\ u(x, 0) = u_0(x), & x \in \mathbb{R}. \end{cases}$$

Let us assume that the entropy weak solution of (21) has discontinuities of the simplest kind; namely, we suppose that there is a smooth curve Γ_u , given by $x = x(t)$, such that u is smooth on either side of Γ_u , with a simple jump across Γ_u . Letting u^l and u^r denote the left and right limits of $u(\cdot, t)$, it then follows from the integral identity (14), via Green's formula, that the Rankine-Hugoniot condition holds across the curve Γ_u :

$$(22) \quad s := x'(t) = \frac{f(u^l) - f(u^r)}{u^l - u^r}.$$

The following geometric interpretation of the Kruřkov entropy condition (17) is known as Oleřnik's theorem or entropy condition [124].

Theorem 3.2 ([124]). *Let $u(x, t)$ be a piecewise smooth solution to (21) with jumps across Γ_u satisfying (22). Then the entropy condition (17) holds if and only if:*

- ($u^r < u^l$): The graph $y = f(u)$ restricted to $[u^r, u^l]$ lies below or equals the chord connecting the point $(u^r, f(u^r))$ to the point $(u^l, f(u^l))$, i.e.,

$$(23) \quad \frac{f(u^l) - f(k)}{u^l - k} \geq s, \quad \forall k \in (u_r, u_l).$$

- ($u^r > u^l$): The graph $y = f(u)$ restricted to $[u^l, u^r]$ lies above or equals the chord connecting the point $(u^l, f(u^l))$ to the point $(u^r, f(u^r))$, i.e.,

$$(24) \quad \frac{f(u^r) - f(k)}{u^r - k} \leq s, \quad \forall k \in (u_l, u_r).$$

Remark 3.1. *Oleřnik's entropy condition states that the entropy loss associated with a shock in the solution of (21) manifests itself in the form of a local convexification of the flux function. This geometric interpretation of the entropy loss turns out to be the heart of the matter of the corrected operator splitting algorithms described §4.*

We next consider nonlinear convection-diffusion problems of the form

$$(25) \quad \begin{cases} \partial_t u + \nabla \cdot f(u) = \nabla \cdot (d(u)\nabla u) = \Delta D(u), & (x, t) \in \Pi_T = \mathbb{R}^m \times (0, T), \quad m \geq 1, \\ u(x, 0) = u_0(x), & x \in \mathbb{R}^m, \end{cases}$$

where $f = (f_1, \dots, f_m)$ is the convection flux and $D(u)$ is the diffusion function

$$(26) \quad D(u) = \int_0^u d(\xi) d\xi.$$

If not otherwise stated, it is always understood that the functions f, D are sufficiently smooth and that u_0 (at least) belongs to $L^1 \cap L^\infty \cap BV$. The L^1/BV solution theory presented below can, of course, be extended to more general convection-diffusion equations with variable coefficients, a source term, and a second order diffusion term containing mixed partial derivatives.

Let us first assume that the convection-diffusion equation is uniformly parabolic, i.e.,

$$(27) \quad d(\xi) \geq \gamma > 0, \quad \forall \xi.$$

With a solution of (25) we then understand a function $u(x, t)$ which is at least twice continuously differentiable in x and at least once in t such that the partial differential equation is satisfied in the classical sense for $t > 0$. Furthermore, we require that $u(t) \rightharpoonup u_0$ in the weak sense, i.e.,

$$\int (u(x, t) - u_0(x))\phi(x) dx \rightarrow 0 \text{ as } t \rightarrow 0+, \quad \forall \phi \in C_0(\mathbb{R}^m).$$

It well known that (25) possesses such a solution and that it is unique. We refer to the survey paper of Oleřnik and Kruřkov [125] for a nice overview of the theory of parabolic equations.

For later use, let us collect some important L^1 type estimates not found in [125].

Theorem 3.3. *Let u, v be smooth solutions of the convection-diffusion problems*

$$(28) \quad \partial_t u + \nabla \cdot f(u) = \Delta D(u), \quad u|_{t=0} = u_0,$$

$$(29) \quad \partial_t v + \nabla \cdot g(v) = \Delta D(v), \quad v|_{t=0} = v_0.$$

Then we have

$$(30) \quad \|u(\cdot, T) - v(\cdot, T)\|_{L^1} \leq \|u_0 - v_0\|_{L^1} + T \min(|u_0|_{BV}, |v_0|_{BV}) \max_j \|f_j - g_j\|_{\text{Lip}}.$$

Furthermore, a smooth solution of (25) satisfies the following estimates:

$$(31) \quad \begin{cases} \text{(a)} & \|u(\cdot, t)\|_{L^\infty} \leq \|u_0\|_{L^\infty}, \\ \text{(b)} & |u(\cdot, t)|_{BV} \leq |u_0|_{BV}, \\ \text{(c)} & \|u(\cdot, t_2) - u(\cdot, t_1)\|_{L^1} \leq \text{Const} \cdot \sqrt{|t_2 - t_1|}, \quad \forall t_1, t_2 \geq 0. \end{cases}$$

Remark 3.2. *We will later show that our approximate solutions satisfy estimates very similar to those in (31), which in turn will imply compactness of the numerical approximations. It is important to notice that estimates (a)-(c) in (31) continue to hold in the degenerate case. The fact that these estimates are independent of γ (the lower bound on $d(\cdot)$) makes the L^1 space rather attractive from the point of view of numerical analysis for parabolic equations.*

To prove estimate (c) in (31), we need a version of an interpolation lemma due to Kruřkov [107]. This lemma is also used in §4 for convergence analysis of operator splitting.

Lemma 3.1. *Let there be finite constants C_1, C_2 , and C_3 such that $z : \bar{\Pi}_T \rightarrow \mathbb{R}$ satisfies the two estimates*

$$\begin{aligned} \|z(\cdot, t)\|_{L^\infty} &\leq C_1, & \text{for all } t \in [0, T], \\ |z(\cdot, t)|_{BV} &\leq C_2, & \text{for all } t \in [0, T], \end{aligned}$$

and the weak time estimate

$$\left| \int (z(x, t_2) - z(x, t_1)) \phi(x) dx \right| \leq C_3 (\|\phi\|_{L^\infty} + \max_j \|\phi_{x_j}\|_{L^\infty}) |t_2 - t_1|,$$

for all $\phi \in C_0^1$ and $0 \leq t_1, t_2 \leq T$. Then there is a constant C , depending in particular on C_1 and C_2 , such that the following interpolation result is valid:

$$\|z(\cdot, t_2) - z(\cdot, t_1)\|_{L^1} \leq C \sqrt{|t_2 - t_1|}, \quad 0 \leq t_1, t_2 \leq T.$$

See [100, 99] for a proof of this lemma.

Proof (of Theorem 3.3). The proof of (30) uses a classical dual (error) argument. The quantity $e = v - u$ solves the (error) equation

$$(32) \quad \partial_t e + \nabla \cdot (a(x, t)e) - \Delta(b(x, t)e) = T(x, t),$$

where the vector $a(x, t) = (a_1(x, t), \dots, a_m(x, t))$ and the scalar $b(x, t)$ are given as

$$\begin{aligned} a_j(x, t) &= \frac{f_j(v) - f_j(u)}{v - u}, & j = 1, \dots, m, \\ b(x, t) &= \frac{D(v) - D(u)}{v - u}, \end{aligned}$$

and $T(x, t)$ denotes the truncation error,

$$T(x, t) = \partial_t v + \nabla \cdot f(v) - \Delta D(v).$$

Now, for given $T > 0$, let ψ solve the backward problem

$$(33) \quad \begin{cases} \partial_t \psi + a(x, t) \cdot \nabla \psi + b(x, t) \Delta \psi = 0, & t < T, \\ \psi|_{t=T} = \phi \in C^\infty(\mathbb{R}^m). \end{cases}$$

Then $\psi(t)$ is well defined for $t \leq T$ and the maximum principle yields

$$\|\psi(t)\|_{L^\infty} \leq \|\phi\|_{L^\infty}.$$

By integrating the error equation (32) against ψ over Π_T , and noting that (33) is just the adjoint problem of (32), we obtain (assuming that ϵ decreases rapidly to zero as $|x| \rightarrow \infty$)

$$(34) \quad \int e(x, T)\phi(x) dx = \int e(x, 0)\psi(x, 0) dx + \iint T(x, t)\psi(x, t) dt dx.$$

We are now equipped with the tool (34) needed to prove (30). Assume first $f = g$ so that $T \equiv 0$. Then by choosing $\phi = \text{sign}(e)$ (omitting a standard approximation argument) and using the maximum principle for $\psi(t)$, we obtain

$$(35) \quad \begin{aligned} \int |v(x, T) - u(x, T)| dx &\leq \|\psi(\cdot, 0)\|_{L^\infty} \int |v_0(x) - u_0(x)| dx \\ &\leq \int |v_0(x) - u_0(x)| dx. \end{aligned}$$

Observe now that estimate (b) is a direct consequence of the L^1 contraction property (35) since the convection-diffusion equation (25) is translation invariant.

Equipped with (34) and (35), it remains to estimate the truncation error in (34). Using (b) and again the maximum principle for ψ , we can readily calculate

$$\begin{aligned} \left| \iint T(x, t)\psi(x, t) dt dx \right| &= \left| \iint \nabla \cdot (f(v) - g(v))\psi(x, t) dt dx \right| \\ &\leq \max_j \|f_j - g_j\|_{\text{Lip}} \sum_j \iint |\partial_{x_j} v| |\psi(x, t)| dt dx \\ &\leq T \max_j \|f_j - g_j\|_{\text{Lip}} |v_0|_{BV} \|\phi\|_{L^\infty}. \end{aligned}$$

Choosing $\phi = \text{sign}(e)$ (again omitting a standard approximation argument) in (34), we now obtain

$$\|v(\cdot, T) - u(\cdot, T)\|_{L^1} \leq \|v_0 - u_0\|_{L^1} + T |v_0|_{BV} \max_j \|f_j - g_j\|_{\text{Lip}}.$$

Finally, using symmetry we derive the desired stability result (30).

It remains to prove (a) and (c). The first claim follows from the maximum principle. We are going to use (b) and Lemma 3.1 to derive the time estimate (c). To this end, we shall employ a technique introduced by Kruřkov [107]. Let $\phi(x)$ be a test function on \mathbb{R}^m . Multiplying (25) by ϕ , integrating the result in space, and subsequently integrating by parts, yields

$$\begin{aligned} \left| \int \phi(x) \partial_t u dx \right| &\leq \left| \int f'(u) \cdot \nabla u \phi dx \right| + \left| \int D'(u) \nabla u \cdot \nabla \phi \right| \\ &\leq \text{Const} \cdot (\|\phi\|_{L^\infty} + \max_j \|\partial_{x_j} \phi\|_{L^\infty}), \end{aligned}$$

where the BV estimate (b) has been used. From this estimate we get the following weak continuity result

$$(36) \quad \left| \int (u(x, t_2) - u(x, t_1)) \phi(x) dx \right| \leq \text{Const} \cdot (\|\phi\|_{L^\infty} + \max_j \|\partial_{x_j} \phi\|_{L^\infty}) |t_2 - t_1|.$$

Applying Lemma 3.1 to (36), we get estimate (c). \square

Remark 3.3. *The proof of Theorem 3.3 was based on a classical dual argument. It seems difficult to get a stability result with respect to the diffusion function using this technique. However, Cockburn and Gripenberg [37] have recently obtained such stability using an elegant extension of Kruřkov's "doubling of the variables".*

We now turn our attention to degenerate convection-diffusion equations. To this end, we replace condition (27) by

$$(37) \quad d(\xi) \geq 0, \quad \forall \xi.$$

When (25) is non-degenerate, the equation admits classical solutions. This fact contrasts with the case where (25) is allowed to degenerate ($d(u) = 0$) for some values of u . In general, a striking manifestation of the point degeneracy is the finite speed of propagation of disturbances. Thus, if $d(0) = 0$ and at some fixed time the solution u has compact support, then it will continue to have

compact support for all later times. The transition from a region where $u > 0$ to one where $u = 0$ is not smooth and it is therefore necessary to deal with (continuous) weak solutions rather than classical solutions, see the book [139] (and the references cited therein) for further details.

Recall that the convection-diffusion equations arising in reservoir simulation typically degenerates at two points, see §2. A natural generalisation would be to consider equations for which the function $D(u)$ (see (26)) is strictly increasing in u . Note that a sufficient condition for $D(u)$ to be strictly increasing is that

$$\text{meas}\{\xi : d(\xi) = 0\} = 0,$$

which does not rule out the possibility that $d(u)$ has an infinite number of zero points. To deal with this kind of parabolic degeneracy, we introduce the following notion of a generalised solution:

Definition 3.2. *Suppose that $D(u)$ is strictly increasing. Then a function $u(x, t)$ is called a BV weak solution of the Cauchy problem (25) if:*

1. $u \in L^\infty(\Pi_T) \cap BV(\Pi_T)$ and $\nabla D(u) \in L^2_{\text{loc}}(\Pi_T; \mathbb{R}^n)$.
 2. For all test functions $\phi \in C_0^\infty(\Pi_T)$ such that $\phi|_{t=T} = 0$,
- $$(38) \quad \iint \left(u \partial_t \phi + [f(u) - \nabla D(u)] \cdot \nabla \phi \right) dt dx + \int u_0(x) \phi(x, 0) dx = 0.$$

Provided u_0 is sufficiently smooth, existence of a BV weak solution is established in the work of Vol'pert and Hudjaev [150] by sending ε to zero in the parabolic regularization

$$(39) \quad \partial_t u_\varepsilon + \nabla \cdot f(u_\varepsilon) = \Delta D(u_\varepsilon) + \varepsilon \Delta u_\varepsilon, \quad u_\varepsilon(x, 0) = u_0(x).$$

Yin [163] has proved that BV weak solutions are uniquely determined by their initial data. More precisely, he proved that if u and v are BV weak solutions of (25) with data u_0 and v_0 , respectively, then the L^1 stability result (18) holds. Using the essential condition that $D(\cdot)$ is strictly increasing, the L^1 stability result is proved by showing that the set of discontinuity points of BV weak solutions is of m -dimensional measure zero. Zhao [164] has proved that if (x_0, t_0) is a point of approximate continuity of a BV solution u such that $d(u(x_0, t_0)) > 0$, then u is a classical solution in a neighbourhood of (x_0, t_0) . Furthermore, in one space dimension ($m = 1$), the BV solution is continuous, see [164]. Under the hypothesis

$$D \in C^1(\mathbb{R}), \quad D' > 0 \text{ a.e. in } \mathbb{R} \quad \text{and} \quad |f'|^2 \leq \sigma D', \quad \sigma \in C(\mathbb{R}),$$

Bénilan and Gariépy [12] have shown that the unique BV weak solution of (25) is actually a strong solution, i.e., $\partial_t u$, $\nabla \cdot f(u)$, and $\Delta D(u)$ are functions in $L^1_{\text{loc}}(\Pi_T)$ (and not merely locally finite measures on Π_T). Zhao [166] has shown recently that the requirement $u \in BV(\Pi_T)$ in Definition 3.2 can be replaced by the weaker requirement $u \in BV_x(\Pi_T)$, where $BV_x(\Pi_T) \supset BV(\Pi_T)$ denotes the space consisting of locally integrable functions $z(x, t)$ for which $\partial_x z$ is a locally finite measure on Π_T . Note that if $z \in BV_x(\Pi_T)$, then $z(\cdot, t) \in BV(\mathbb{R})$ for a.e. $t \in (0, T)$.

Equipped with Theorem 3.3 and the uniqueness theorem of Yin [163], we can pass to the limit in the parabolic regularization (39) (following [150]) and conclude that the following theorem holds:

Theorem 3.4. *If u and v are BV weak solutions (see Definition 3.2) of (28) and (29), respectively, then (30) holds.*

Bürger et al. [23, 24, 25, 29, 38] have in a series of papers proposed and analysed a sedimentation model which contain a certain nonlinear partial differential equation. This partial differential equation is similar to the saturation equation in the reservoir flow model. However, the main difference is that the diffusion coefficient in the sedimentation model is degenerate on intervals, and not only at isolated points as is the case with the saturation equation (6). The splitting algorithms described in §4 can also be applied to the sedimentation model [27, 28].

We end this section with a discussion of the strongly degenerate case, i.e., the case where $D(u)$ is merely non-decreasing. In this case there exists at least one interval $[\alpha, \beta]$ such that

$$d(\xi) = 0, \quad \forall \xi \in [\alpha, \beta].$$

A simple example of a strongly degenerate equation is a hyperbolic equation. Strongly degenerate equations will in general possess discontinuous solutions. Furthermore, discontinuous weak solutions are not uniquely determined by their data. In fact, an additional condition — the entropy condition — is needed to single out the physically relevant weak solution of the problem. For strongly degenerate equations that possess discontinuous solutions, a natural generalisation of Definition 3.2 is the following:

Definition 3.3. *Suppose that $D(u)$ is non-decreasing. Then a BV weak solution $u(x, t)$ of (25) is called a BV entropy weak solution if, for all non-negative test functions $\phi \in C_0^\infty(\Pi_T)$ and $k \in \mathbb{R}$,*

$$(40) \quad \iint \left(|u - k| \partial_t \phi + \text{sign}(u - k) [f(u) - f(k) - \nabla D(u)] \cdot \nabla \phi \right) dt dx \geq 0.$$

Remark 3.4. *In the one-dimensional case, the condition $\partial_x D(u) \in L_{loc}^2(\Pi_T)$ can be replaced by the stronger condition $D(u) \in C^{1, \frac{1}{2}}(\Pi_T)$, where $C^{1, \frac{1}{2}}(\Pi_T)$ denotes the space of functions that are Hölder continuous with exponent 1 in the space variable and 1/2 in the time variable.*

Note that the entropy condition (40) reduces to Kružkov's entropy condition (17) for hyperbolic problems when $d \equiv 0$, and thus Definition 3.3 contains the hyperbolic problem (13) as a special case. This condition was first proposed by Vol'pert and Hudjaev [150], who also showed, provided u_0 is sufficiently smooth, existence of a BV entropy weak solution by passing to the limit in the parabolic regularization (39). It is easy to see that the entropy condition (40) implies that the partial differential equation in (25) holds in the distributional sense. Consequently, the generalised derivative $\Delta D(u)$ is a locally finite measure on Π_T , since $\partial_t u$ and $\nabla \cdot f(u)$ are locally finite measures, and the partial differential equation in (25) holds in the sense of equality of measures.

In the one-dimensional case, Wu and Yin [160] have proved uniqueness of BV entropy weak solutions. More precisely, they have proven that if u and v are BV entropy weak solutions with initial data u_0 and v_0 , respectively, then (18) holds. For further results — via nonlinear semigroup theory — on existence, uniqueness and continuous dependence on the data of entropy solutions in the one-dimensional case, we refer to Bénilan and Touré [14, 15, 16]. Some partial uniqueness results for generalised solutions of multi-dimensional problems are obtained in Brézis and Crandall [21] and in the recent work of Carrillo [32]. Existence and uniqueness results for various initial-boundary value problems can be found in [26, 30, 157, 158, 159, 161, 165].

The uniqueness proof of Wu and Yin [160] is based on a characterisation of the set of discontinuity points of u (the jump conditions). In [160], the authors corrected a previous result by Vol'pert and Hudjaev [150] stating that the jump conditions for strongly degenerate parabolic equations coincide with the jump conditions for purely hyperbolic equations. Before stating the (correct) jump conditions, we must introduce some notation. Let Γ_u be the set of jumps, that is; $(x_0, t_0) \in \Gamma_u$ if and only if there exists a unit vector $\nu = (\nu_t, \nu_x)$ such that the approximate limits of u at (x_0, t_0) from the sides of the half-planes $(t - t_0)\nu_t + (x - x_0)\nu_x < 0$ and $(t - t_0)\nu_t + (x - x_0)\nu_x > 0$, denoted by $u^-(x_0, t_0)$ and $u^+(x_0, t_0)$, respectively, exist and are not equal. Similarly, let $u^l(x, t)$ and $u^r(x, t)$ denote the left and right approximate limits of $u(\cdot, t)$ respectively. One should note the difference between u^-, u^+ and u^l, u^r . The approximate limits u^-, u^+ are well-defined for $u \in BV(\Pi_T)$ while the limits u^l, u^r exist under the weaker assumption $u \in BV_x(\Pi_T)$. Introduce the notations $\text{sign}^+ := \text{sign}$ and $\text{sign}^- := \text{sign}^+ - 1$, and let $\text{int}(a, b)$ denote the closed interval bounded by a and b . Finally, let H_1 denote the one-dimensional Hausdorff measure.

Theorem 3.5 ([160]). *Let $u(x, t)$ be a BV entropy weak solution (see Definition 3.3) of (25) with $m = 1$. Then H_1 - almost everywhere on Γ_u , we have:*

$$(41) \quad d(k) = 0, \quad \forall k \in \text{int}(u^-, u^+), \quad \nu_x \neq 0.$$

$$(42) \quad (u^+ - u^-)\nu_t + (f(u^+) - f(u^-))\nu_x - (\partial_x D(u)^r - \partial_x D(u)^l)|\nu_x| = 0.$$

For all $k \in \mathbb{R}$,

$$(43) \quad \begin{aligned} & |u^+ - k|\nu_t + \text{sign}(u^+ - k)[f(u^+) - f(k) - (\partial_x D(u)^r \text{sign}^+ \nu_x - \partial_x D(u)^l \text{sign}^- \nu_x)]\nu_x \\ & \leq |u^- - k|\nu_t + \text{sign}(u^- - k)[f(u^-) - f(k) - (\partial_x D(u)^l \text{sign}^+ \nu_x - \partial_x D(u)^r \text{sign}^- \nu_x)]\nu_x. \end{aligned}$$

Conditions (42) and (43) are, respectively, generalisations of the Rankine-Hugoniot condition (22) and Oleinik's entropy condition (see Theorem 3.2) for conservation laws. One should observe that for the multi-dimensional case, it is not possible to conclude from the Definition 3.3 that each $\partial_x D_j(u)$ is a finite measure on Π_T , although $\Delta D(u)$ is. This fact prevents one from deriving the analogue of the jump conditions — and thus L^1 stability — in the multi-dimensional case, although the BV_x theory of Wu and Yin [160] can be extended to the multi-dimensional case.

We next note that the jump conditions (42) and (43) can be more instructively stated as follows (see [65] for a proof):

Corollary 3.1. *Let $u(x, t)$ be a piecewise smooth BV entropy weak solution (see Definition 3.3) of (25) with $m = 1$. Assume that $d(k) = 0$ for all $k \in [u_*, u^*]$ for some $u_*, u^* \in \mathbb{R}$. A jump between two values u^l and u^r of the solution $u(x, t)$, which is referred to as a shock, can occur only for $u^l, u^r \in [u_*, u^*]$. This shock must satisfy:*

1. The shock speed s is given by

$$(44) \quad s = \frac{f(u^r) - f(u^l) - (\partial_x D(u)^r - \partial_x D(u)^l)}{u^r - u^l}.$$

2. For all $k \in \text{int}(u^l, u^r)$, the following entropy condition holds:

$$(45) \quad \frac{f(u^r) - f(k) - \partial_x D(u)^r}{u^r - k} \leq s \leq \frac{f(u^l) - f(k) - \partial_x D(u)^l}{u^l - k}.$$

It is important to realize that solutions of strongly degenerate parabolic equations in general have a more complex structure than solutions of hyperbolic equations. The following example demonstrates this.

Example 3.1 (Structure of Solutions). *This example is taken from Evje and Karlsen [65]. We consider the Burgers type equation*

$$(46) \quad \partial_t u + \partial_x(u^2) = \partial_x(d(u)\partial_x u),$$

where

$$(47) \quad d(u) = \begin{cases} 0, & \text{for } x \in [0, 0.5], \\ 2.5u - 1.25, & \text{for } x \in [0.5, 0.6], \\ 0.25, & \text{for } x \in [0.6, 1]. \end{cases}$$

Note that $d(\cdot)$ is continuous and degenerates on the interval $[0, 0.5]$. In Figure 2 we have plotted the initial function, the solution of the corresponding conservation law, i.e., $d \equiv 0$ in (46), and the solution of (46) at time $T = 0.15$. A finite difference method (with very fine discretization parameters) is used to compute the solutions. An interesting observation is that the solution of (46) has a "new" increasing jump, despite of the fact that f is convex. Thus the solution is not bounded in the Lip^+ norm, as opposed to the solution of the conservation law (see [142]). Moreover, while the speed of a jump in the conservation law solution is determined solely by f (see Theorem 3.2), the speed of a jump in the solution of (46) is in general determined by the jumps in both $f(u)$ and $\partial_x D(u)$ (see Corollary 3.1). In Figure 3, we have given a geometric interpretation of the entropy condition (45) for the solution shown in Figure 2 (right), which possesses two shocks. (i) Left shock: note that $\partial_x D(u)^l = 0$ and $\partial_x D(u)^r > 0$, see Figure 2 (right). Condition (45) states that the graph of f restricted to the interval $[u^l, u^r]$ lies above or equals the straight line between $(u^l, f(u^l))$ and $(u^r, f(u^r) - \partial_x D(u)^r)$, see Figure 3 (left). (ii) Right shock: note that $\partial_x D(u)^l < 0$ and $\partial_x D(u)^r = 0$. Condition (45) now states that the graph of f restricted to $[u^r, u^l]$ lies below or equals the straight line between $(u^r, f(u^r))$ and $(u^l, f(u^l) - \partial_x D(u)^l)$, see Figure 3 (right).

The BV solution theory can be generalised to doubly nonlinear degenerate parabolic equations of the form

$$(48) \quad \partial_t u + \partial_x f(u) = \partial_x \mathcal{A}(d(u)\partial_x u), \quad \mathcal{A}(\pm\infty) = \pm\infty, \mathcal{A}'(s) \geq 0, d(s) \geq 0.$$

The functions $\mathcal{A}'(s)$ and $d(s)$ are allowed to have an infinite number of degenerate intervals in \mathbb{R} . Included in (48) are equations arising from the theory of non-Newtonian fluids. We say that $u(x, t)$ is a BV entropy weak solution of the Cauchy problem for (48) if:

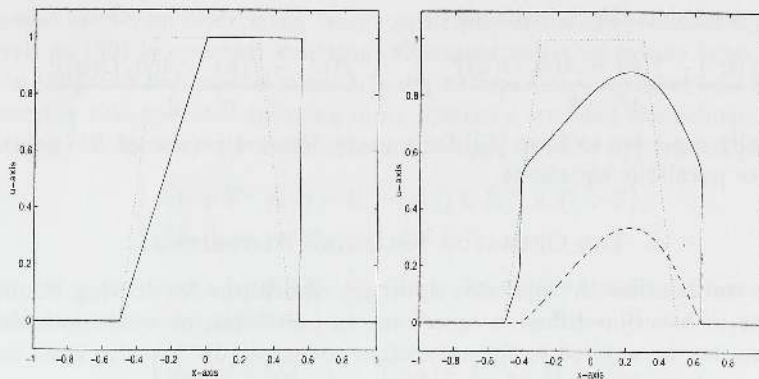


FIGURE 2. Left: The solution (solid) of the inviscid Burgers type equation. Right: The solution (solid) of the Burgers type equation with a strongly degenerate diffusion term and the corresponding diffusion function $D(u(\cdot, t))$ (dashed). The initial function is shown as dotted.

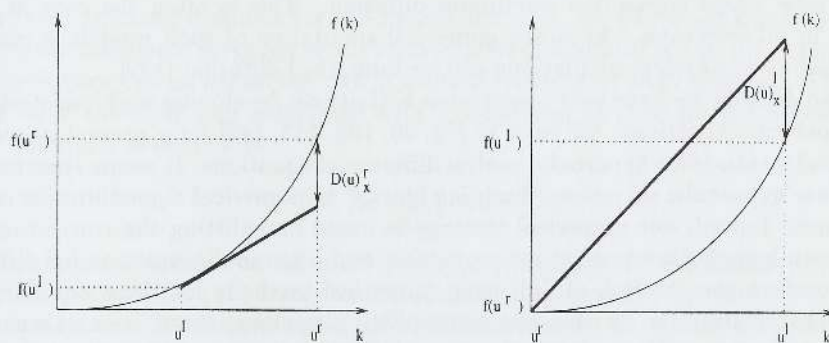


FIGURE 3. Geometric interpretation of the entropy condition (45) for the solution shown in Figure 2 (right).

1. $u \in L^\infty(\Pi_T) \cap BV(\Pi_T)$ and $D(u) \in C^{1, \frac{1}{2}}(\bar{\Pi}_T)$.
2. For all non-negative $\phi \in C_0^\infty(\Pi_T)$ such that $\phi|_{t=T} = 0$ and $k \in \mathbb{R}$,

$$\iint \left(|u - k| \partial_t \phi + \text{sign}(u - k) [f(u) - f(k) - \mathcal{A}(\partial_x D(u))] \partial_x \phi \right) dt dx + \int |u_0(x) - k| \phi(x, 0) dx \geq 0.$$

We refer to Yin [162] for a treatment of the initial-boundary value problem for (48). Yin uses the method of parabolic regularization for the existence proof. Evje and Karlsen [64] have treated the Cauchy problem for (48) using finite difference methods. Yin [162] has used the BV_x theory [160] to derive the jump conditions — and thus L^1 stability — for discontinuous solutions of doubly nonlinear problems. Without going into details, we only mention that for doubly nonlinear problems the shock speed (44) is replaced by

$$s = \frac{f(u^r) - f(u^l) - (\mathcal{A}(\partial_x D(u))^r - \mathcal{A}(\partial_x D(u))^l)}{u^r - u^l},$$

while the entropy condition (45) is replaced by

$$(49) \quad \frac{f(u^r) - f(k) - \mathcal{A}(\partial_x D(u))^r}{u^r - k} \leq s \leq \frac{f(u^l) - f(k) - \mathcal{A}(\partial_x D(u))^l}{u^l - k},$$

see also [64]. Finally, we refer to Evje [62] for a more detailed review of BV solution theory for strongly degenerate parabolic equations.

4. THE OPERATOR SPLITTING ALGORITHMS

In this section we describe the operator splitting algorithms for solving nonlinear, possibly strongly degenerate, convection-diffusion equations. In particular, as we demonstrate in §7, these splitting algorithms can be applied to the saturation equation (6). We also state and prove some typical convergence results for some of the splitting algorithms. Performance results for several nonlinear model problems are presented, and the importance of having a “correction strategy” for reducing splitting errors is illustrated. The correction strategy that we employ is described in detail. For clarity of presentation, we mainly present and analyse the operator splitting algorithms in their semi-discrete form for a simplified convection-diffusion problem. For numerical purposes, we use fully discrete splitting algorithms based on the (large time step) hyperbolic solvers described in §5 and the parabolic solvers described in §6.

It is well known that accurate modelling of convective and diffusive processes is one of the most challenging tasks in the numerical approximation of partial differential equations. Particularly difficult is the case where convection dominates diffusion. This is often the case in models of two-phase flow in oil reservoirs. Accurate numerical simulation of such models is consequently often complicated by unphysical oscillations and/or numerical diffusion [122].

In the last two decades we have seen an enormous activity on developing sophisticated numerical methods for hyperbolic equations. We refer to [79, 90, 105, 113, 146] for a general introduction to modern numerical methods for hyperbolic partial differential equations. It seems reasonable to employ some of these hyperbolic solvers as “building blocks” in numerical algorithms for convection-diffusion problems. Indeed, our numerical strategy is based on splitting the convection-diffusion equation (6) into a hyperbolic equation for convection and a parabolic equation for diffusion. We then try to reproduce the solution of (6) using numerical methods for these simpler equations as building blocks. Variations on this operator splitting approach have been taken in various contexts by many authors. The novelty of our work lies in the use of large time step methods for the convection step and a correction strategy (or an appropriate flux splitting) for reducing potential splitting errors. Applying large time step algorithms for the convection step has some advantages. In particular, equipped with an implicit diffusion solver, the resulting operator splitting algorithms are unconditionally stable in the sense that there is no CFL condition restricting the time step. However, it turns out that a reasonable choice of time step is highly dictated by the degree of (nonlinear) interplay between convective and diffusive forces. In particular, large time steps can lead to fronts that are too wide. However, as we will see later, it is possible to identify and correct (or counterbalance) this nonlinear splitting error so that correct width of fronts is ensured also when the time steps are large. We refer to the books [122, 135] for an introduction to more standard numerical algorithms for convection-diffusion problems.

For simplicity of presentation, we restrict our attention to convection-diffusion problems of the form

$$(50) \quad \begin{cases} \partial_t u + \nabla \cdot f(u) = \varepsilon \Delta u, & (x, t) \in \Pi_T = \mathbb{R}^m \times (0, T), \quad m \geq 1, \\ u(x, 0) = u_0(x), & x \in \mathbb{R}^m, \end{cases}$$

where the flux vector $f = (f_1, \dots, f_m)$ is sufficiently smooth and the initial function u_0 belongs to $L^1 \cap L^\infty \cap BV$. We emphasise that the numerical solution algorithms and their convergence analysis presented below carry over to more general convection-diffusion equations with variable coefficients, a source term, and a second order diffusion term containing mixed partial derivatives. Also, due to space limitation, we only treat the Cauchy problem. Details on the extension of the operator splitting algorithms to various boundary value problems can be found in [27, 97].

As was discussed above, an underlying design principle for many successful solution algorithms for problems such as (50) is operator splitting. Operator splitting means here that we split the time evolution in (50) into two partial steps in order to separate out the effects of convection and diffusion. To describe this operator splitting more precisely, we need the solution operator taking the initial data $v_0(x)$ to the entropy weak solution at time t of the hyperbolic problem

$$(51) \quad \begin{cases} \partial_t v + \nabla \cdot f(v) = 0, & (x, t) \in \mathbb{R}^m \times \{t > 0\}, \\ v(x, 0) = v_0(x), & x \in \mathbb{R}^m. \end{cases}$$

This solution operator we denote by $\mathcal{S}^f(t)$. Similarly, let $\mathcal{H}(t)$ be the solution operator (at time t) associated with the parabolic problem

$$(52) \quad \begin{cases} \partial_t w = \varepsilon \Delta w, & (x, t) \in \mathbb{R}^m \times \{t > 0\}, \\ w(x, 0) = w_0(x), & x \in \mathbb{R}^m. \end{cases}$$

Now fix $T > 0$ and $\Delta t > 0$, and let N be such that $N\Delta t = T$. Furthermore, let $t_n = n\Delta t$ for $n = 0, \dots, N$ and $t_{n+1/2} = (n + \frac{1}{2})\Delta t$ for $n = 0, \dots, N - 1$. We then let the operator splitting solution $u_{\Delta t}$ be defined at the discrete times $t_n = n\Delta t$ by the product formula

$$(53) \quad u_{\Delta t}(x, n\Delta t) = [\mathcal{H}(\Delta t) \circ \mathcal{S}^f(\Delta t)]^n u_0(x).$$

In applications, the exact solution operators $\mathcal{S}^f(t)$ and $\mathcal{H}(t)$ are replaced by appropriate numerical approximations. We use the modified method of characteristics (together with a suitable flux splitting) or front tracking methods for the hyperbolic part, see §5 for details. For the parabolic part we use finite difference methods or a Petrov-Galerkin method, see §6 for details.

For later reference, let us define the CFL (Courant-Friedrichs-Lewy) number. If Δx is the grid spacing and Δt is the time step associated with a numerical method for the hyperbolic problem (51), the CFL number is defined as

$$(54) \quad \text{CFL} := \max_u |f'(u)| \frac{\Delta t}{\Delta x},$$

where the maximum is taken over all u in $[-\|u_0\|_{L^\infty}, \|u_0\|_{L^\infty}]$. The classical CFL condition for finite difference methods for (51) states that (54) should be bounded by one.

Here we mention that Dawson, Wheeler, and collaborators [50, 51, 52, 53, 156] are using operator splitting algorithms similar to (53). In their splitting algorithm, the hyperbolic equation (51) is solved by $M \geq 1$ local time steps (for each global splitting step) with an explicit high resolution Godunov type method, while the diffusion equation (52) is solved implicitly. The point is that such splitting algorithms may be more efficient than standard numerical methods when $M > 1$, since the implicit equations need not be solved during each update of the conservation law. Since the explicit nature of the convection solver requires a CFL time step constraint, the basic splitting procedure may be expensive, especially if the CFL constraint is severe. Different from the view taken by Dawson et al., we also insist on using large time step methods for the convection updates, i.e., methods that avoid a CFL constraint. We will come back to this point later when discussing the corrected operator splitting algorithms.

Note that we have only defined $u_{\Delta t}$ at the discrete times t_n . In between two consecutive discrete times, we use the following time interpolant:

$$(55) \quad u_{\Delta t}(x, t) = \begin{cases} \mathcal{S}^f(2(t - t_n))u^n, & t \in (t_n, t_{n+1/2}], \\ [\mathcal{H}(2(t - t_{n+1/2})) \circ \mathcal{S}^f(\Delta t)]u^n, & t \in (t_{n+1/2}, t_{n+1}], \end{cases}$$

where $u^n = u_{\Delta t}(t_n)$. Regarding $u_{\Delta t}$ we have the following lemma:

Lemma 4.1 ([100]). *The following a priori estimates hold:*

$$(56) \quad \begin{cases} (a) & \|u_{\Delta t}(\cdot, t)\|_{L^\infty} \leq \|u_0\|_{L^\infty}, \\ (b) & |u_{\Delta t}(\cdot, t)|_{BV} \leq |u_0|_{BV}, \\ (c) & \|u_{\Delta t}(\cdot, t_2) - u_{\Delta t}(\cdot, t_1)\|_{L^1} \leq \text{Const} \cdot \sqrt{|t_2 - t_1|}, \quad \forall t_1, t_2 \geq 0. \end{cases}$$

Proof. Claim (a) is true because the solution operators $\mathcal{S}^f(t)$ and $\mathcal{H}(t)$ do not introduce new minima or maxima. Similarly, claim (b) is true since the solution operators $\mathcal{S}^f(t)$ and $\mathcal{H}(t)$ do not increase the total variation of their initial data.

Fix a test function $\phi \in C_0^\infty(\mathbb{R}^m)$. Using estimate (c) in (20), we get

$$(57) \quad \left| \int (\mathcal{S}^f(t_2)v_0 - \mathcal{S}^f(t_1)v_0)\phi \, dx \right| \leq \text{Const} \cdot \|\phi\|_{L^\infty} |t_2 - t_1|.$$

Using the differential equation for $w(x, t) = \mathcal{H}(t)w_0(x)$ and integration by parts, we get the bound

$$(58) \quad \left| \int (\mathcal{H}(t_2)w_0 - \mathcal{H}(t_1)w_0)\phi \, dx \right| = \left| \int \left(\int_{t_1}^{t_2} \varepsilon \Delta w(x, t) \, dt \right) \phi \, dx \right| \\ \leq \text{Const} \cdot \max_j \|\phi_{x_j}\|_{L^\infty} |t_2 - t_1|.$$

Using (55), (57), and (58), we now readily compute

$$(59) \quad \left| \int (u_{\Delta t}(x, t_2) - u_{\Delta t}(x, t_1))\phi \, dx \right| \leq \text{Const} \cdot (\|\phi\|_{L^\infty} + \max_j \|\phi_{x_j}\|_{L^\infty}) |t_2 - t_1|.$$

Finally, applying Lemma 3.1 to (59) yields estimate (c). \square

In view of estimates (a) and (b) in (56), a classical application of Helly's theorem yields the existence of a subsequence $\{u_{\Delta t_j}(\cdot, t)\}$ converging in L^1_{loc} to a function $u(\cdot, t)$ in $L^\infty \cap BV$ for each fixed t . By a diagonalization argument we obtain the existence of a further subsequence, still denoted by $\{u_{\Delta t_j}(\cdot, t)\}$, which converges for all t in some dense countable subset of $(0, T)$. By appealing to (c), we obtain convergence for all t in $(0, T)$. Summing up, for any given sequence $\{\Delta t\}$ tending to zero, there exists a subsequence $\{\Delta t_j\}$ and a limit function u such that

$$(60) \quad u_{\Delta t_j} \rightarrow u \text{ in } L^1_{loc}(\Pi_T) \text{ as } j \rightarrow \infty.$$

We now prove our main convergence theorem:

Theorem 4.1 ([100]). *Suppose $u_0 \in L^1 \cap L^\infty \cap BV$. Then the operator splitting solution $u_{\Delta t}$ converges in $L^1_{loc}(\Pi_T)$ to the unique classical solution of the Cauchy problem (50) as $\Delta t \rightarrow 0$.*

Proof. We will show that the limit in (60) is a weak solution of (50). To this end, fix a test function $\phi \in C_0^\infty(\mathbb{R} \times [0, T])$ such that $\phi|_{t=T} = 0$, and define a new test function by

$$\varphi(x, t) = \phi\left(x, \frac{t}{2}\right).$$

Let

$$v^n(t) = \mathcal{S}^f(t)u^n, \quad t \in (0, \Delta t).$$

Since $v^n(t)$ satisfies the hyperbolic problem (51) in the sense of distributions on $\mathbb{R}^m \times (0, \Delta t)$ with initial data u^n , the following integral equality holds

$$(61) \quad \int \int_{t_n}^{t_{n+1/2}} \left(\frac{1}{2} u_{\Delta t} \partial_t \phi + f(u_{\Delta t}) \cdot \nabla \phi \right) dt dx \\ = \frac{1}{2} \int \int_0^{\Delta t} \left(v^n(\tau) \partial_\tau \varphi(x, \tau + 2t_n) + f(v^n(\tau)) \cdot \nabla \varphi(x, \tau + 2t_n) \right) d\tau dx \\ = \frac{1}{2} \int u^{n+1/2} \phi(x, t_{n+1/2}) \, dx - \frac{1}{2} \int u^n \phi(x, t_n) \, dx,$$

where we have used the substitution $\tau = 2(t - t_n)$ and introduced the short-hand notation $u^{n+1/2} = \mathcal{S}^f(\Delta t)u^n$. Similarly, let

$$w^n(t) = \mathcal{H}(t)u^{n+1/2}, \quad t \in (0, \Delta t).$$

Since $w^n(t)$ satisfies the parabolic problem (52) in the sense of distributions on $\mathbb{R}^m \times (0, \Delta t)$ with initial data $u^{n+1/2}$, the following integral equality holds

$$\begin{aligned}
 & \int \int_{t_{n+1/2}}^{t_{n+1}} \left(\frac{1}{2} u_{\Delta t} \partial_t \phi + \varepsilon u_{\Delta t} \Delta \phi \right) dt dx \\
 (62) \quad &= \frac{1}{2} \int \int_0^{\Delta t} \left(w^n(\tau) \partial_\tau \varphi(x, \tau + 2t_{n+1/2}) + \varepsilon w_n(\tau) \Delta \varphi(x, \tau + 2t_{n+1/2}) \right) d\tau dx \\
 &= \frac{1}{2} \int u^{n+1} \phi(x, t_{n+1}) dx - \frac{1}{2} \int u^{n+1/2} \phi(x, t_{n+1/2}) dx,
 \end{aligned}$$

where we have used the substitution $\tau = 2(t - t_{n+1/2})$. Adding together (61) and (62), multiplying with 2, and summing the result over all $n = 0, \dots, N-1$, where $N\Delta t = T$, yields

$$\begin{aligned}
 (63) \quad & \sum_{n=0}^{N-1} \int \int_{t_n}^{t_{n+1}} \left(u_{\Delta t} \partial_t \phi + 2\chi_n f(u_{\Delta t}) \cdot \nabla \phi + \varepsilon 2(1 - \chi_n) u_{\Delta t} \Delta \phi \right) dt dx \\
 & + \int u_0(x) \phi(x, 0) dx = 0,
 \end{aligned}$$

where $\chi_n = \chi_n(x, t)$ is the characteristic function of the set $\mathbb{R}^m \times [t_n, t_{n+1/2}]$. Since $\chi_n(x, t) \rightarrow \frac{1}{2}$ in $L^2(\Pi_T)$, we can pass to the limit in (63) and obtain

$$(64) \quad \mathcal{L}(u; \phi) := \iint \left(u \partial_t \phi + f(u) \cdot \nabla \phi + \varepsilon u \Delta \phi \right) dt dx + \int u_0(x) \phi(x, 0) dx = 0.$$

Since ϕ was arbitrary, it follows that the limit u is a weak solution of the Cauchy problem (50). Finally, following Oleřnik [124], we can actually show that this weak solution is a classical solution possessing the necessary smoothness for $t > 0$. This concludes the proof. \square

The analysis presented above is due to Karlsen and Risebro [100]. A refined analysis can be found in [99, 66, 87]. The refined analysis shows that the weak truncation error $|\mathcal{L}(u; \phi)|$ (see (64)) is of order $\mathcal{O}(\sqrt{\Delta t})$ when $u_0 \in BV$. For a sufficiently smooth initial function, it is possible to improve this to $|\mathcal{L}(u; \phi)| = \mathcal{O}(\Delta t)$, see [27]. Karlsen and Lie [96] have analysed operator splitting for convection-diffusion equations with variable coefficients and a source term. Similar convergence results hold for fully discrete operator splitting algorithms. For example, we can replace the hyperbolic solution operator $\mathcal{S}^f(t)$ by front tracking and the parabolic solution operator $\mathcal{H}(t)$ by an explicit or implicit central difference method, see, e.g., [96, 100] for details.

Remark 4.1. *It should be noted that if the numerical method for $\mathcal{H}(t)$ is chosen properly, our numerical solution algorithm is unconditionally stable in the sense that the time step Δt is not limited by the space discretization Δx , i.e., no CFL type condition is associated with the algorithm. Hence, whenever the “physics” of the problem allows for it, large time steps can be used in the simulations.*

Let us for a while restrict our attention to the one-dimensional convection-diffusion problem

$$(65) \quad \partial_t u + \partial_x f(u) = \varepsilon \partial_x (d(u) \partial_x u), \quad u(x, 0) = u_0(x),$$

where also a nonlinear diffusion function $d(\cdot) \geq 0$ has been included. The standard operator splitting algorithm for (65) takes the form

$$(66) \quad u_{\Delta t}(x, n\Delta t) = [\mathcal{H}(\Delta t) \circ \mathcal{S}^f(\Delta t)]^n u_0(x)$$

where $\mathcal{S}^f(t)$ is the solution operator of the hyperbolic equation

$$(67) \quad \partial_t v + \partial_x f(v) = 0,$$

and $\mathcal{H}(t)$ is the solution operator of the parabolic equation

$$(68) \quad \partial_t w = \varepsilon \partial_x (d(w) \partial_x w).$$

Evje and Karlsen [66] have analysed operator splitting for nonlinear, possibly strongly degenerate, convection-diffusion initial value problems, see also [87]. A similar analysis can be found

in Bürger, Evje, and Karlsen [27] for various initial-boundary value problems. The analysis in the degenerate case is similar to the one presented above. Of course, in the case of parabolic degeneracy, we have to show that the approximate solution $u_{\Delta t}$ defined in (66) converges to a limit function u that satisfies the conditions of Definition 3.2, or Definition 3.3 in the case of strong degeneracy. We will not go into all details about the analysis of (66) in the (strongly) degenerate case, see instead [66]. Here we only discuss the condition

$$(69) \quad \partial_x D(u) \in L^2_{\text{loc}}(\Pi_T),$$

where $D(\cdot)$ is defined in (26). Suppose $u_{\Delta t} \rightarrow u$ in $L^1_{\text{loc}}(\Pi_T)$ as $\Delta t \rightarrow 0$. Then we would like to show that u satisfies condition (69). Below we sketch an argument which leads to (69) under the assumption that all functions are sufficiently regular. For details in the general (non-smooth) case, we refer to [66].

Introduce the two sequences $\{\tilde{u}_{\Delta t}\}$ and $\{g_{\Delta t}\}$,

$$\begin{cases} \tilde{u}_{\Delta t}(x, t) = [\mathcal{H}(t - t_n) \circ \mathcal{S}^f(\Delta t)] u^n, & (x, t) \in \mathbb{R} \times (t_n, t_{n+1}), \\ g_{\Delta t}(x, t) = \sqrt{\varepsilon d(\tilde{u}_{\Delta t})} \partial_x \tilde{u}_{\Delta t}, & (x, t) \in \mathbb{R} \times (t_n, t_{n+1}). \end{cases}$$

Since obviously

$$\|u_{\Delta t}(\cdot, t) - \tilde{u}_{\Delta t}(\cdot, t)\|_{L^1} = \mathcal{O}(\sqrt{\Delta t}),$$

we conclude that

$$\tilde{u}_{\Delta t} \rightarrow u \text{ in } L^1_{\text{loc}}(\Pi_T) \text{ as } \Delta t \rightarrow 0.$$

Multiplying the equation for $\tilde{u}_{\Delta t}$ on $\mathbb{R} \times (t_n, t_{n+1})$ by $\tilde{u}_{\Delta t}$, integrating over Π_T , and then integrating by parts in space, we get (recall that $u^{n+1/2} = \mathcal{S}^f(\Delta t)u^n$)

$$\begin{aligned} \|g_{\Delta t}\|_{L^2}^2 &= \iint \varepsilon d(\tilde{u}_{\Delta t}) (\partial_x \tilde{u}_{\Delta t})^2 dt dx = - \iint \varepsilon \partial_x (d(\tilde{u}_{\Delta t}) \partial_x \tilde{u}_{\Delta t}) \tilde{u}_{\Delta t} dt dx \\ &= - \iint \frac{1}{2} \partial_t (\tilde{u}_{\Delta t})^2 dt dx = - \frac{1}{2} \sum_{n=0}^{N-1} \int \left((\tilde{u}_{\Delta t}|_{t=t_{n+1}})^2 - (\tilde{u}_{\Delta t}|_{t=t_n})^2 \right) dx \\ &= - \frac{1}{2} \sum_{n=0}^{N-1} \int \left([(u^{n+1})^2 - (u^n)^2] + [(u^n)^2 - (u^{n+1/2})^2] \right) dx \\ &= - \frac{1}{2} \int_{\mathbb{R}} [(u^N)^2 - (u^0)^2] dx + \frac{1}{2} \sum_{n=0}^{N-1} \int_{\mathbb{R}} [(u^{n+1/2})^2 - (u^n)^2] dx =: I_1 + I_2, \end{aligned}$$

where we have, without loss of generality, assumed that $(d(\tilde{u}_{\Delta t}) \partial_x \tilde{u}_{\Delta t}) \tilde{u}_{\Delta t} \rightarrow 0$ as $|x| \rightarrow \infty$.

Since the operators $\mathcal{S}^f(t)$ and $\mathcal{H}(t)$ both are L^1 contractive, we know that $\|\tilde{u}_{\Delta t}(\cdot, t)\|_{L^1} \leq \|\tilde{u}_{\Delta t}(\cdot, 0)\|_{L^1}$. Thus since $\tilde{u}_{\Delta t}$ is uniformly bounded and the initial function is integrable, the first term is clearly bounded independent of Δt ,

$$(70) \quad |I_1| \leq 2 \|u^0\|_{L^\infty} \|u^0\|_{L^1} = \mathcal{O}(1).$$

Exploiting the L^1 Lipschitz continuity of $\mathcal{S}^f(t)$ and again that $\tilde{u}_{\Delta t}$ is bounded, we obtain for the second term that

$$(71) \quad |I_2| \leq \|u_0\|_{L^\infty} \sum_{n=0}^{N-1} \|\mathcal{S}^f(\Delta t)u^n - u^n\|_{L^1} = \mathcal{O}(1)T.$$

From (70) and (71) we conclude that the following $L^2(\Pi_T)$ bound is valid

$$(72) \quad \|g_{\Delta t}\|_{L^2} \leq M(T),$$

where $M(T)$ is a finite constant independent of η . By virtue of (72) we conclude that $\{g_{\Delta t}\}$ is weakly compact in $L^2_{\text{loc}}(\Pi_T)$. Without loss of generality, we may assume that the entire sequence

$\{g_{\Delta t}\}$ converges weakly in $L^2_{\text{loc}}(\Pi_T)$ to a function g . Let G be defined such that $\partial G(u)/\partial u = \sqrt{\varepsilon d(u)}$ and let ϕ be a test function. We can then calculate

$$\begin{aligned} \iint g(x, t)\phi(x, t) dt dx &= \lim_{\Delta t \rightarrow 0} \iint \partial_x G(\tilde{u}_{\Delta t})\phi dt dx = \lim_{\Delta t \rightarrow 0} \iint (-G(\tilde{u}_{\Delta t})\partial_x \phi) dt dx \\ &= \iint (-G(u)\partial_x \phi) dt dx = \iint \frac{\partial G(u)}{\partial u} \partial_x u \phi dt dx = \iint r(u)\partial_x u \phi dt dx, \quad r(u) = \sqrt{\varepsilon d(u)}. \end{aligned}$$

Consequently, we have shown that $r(u)\partial_x u$ exists in the sense of distributions in $L^2_{\text{loc}}(\Pi_T)$. Finally, from the facts that $u \in L^\infty(\Pi_T)$, $r(u)\partial_x u \in L^2_{\text{loc}}(\Pi_T)$, and (41), we get $d(u)\partial_x u \in L^2_{\text{loc}}(\Pi_T)$, see [150] for details. Thus (69) holds.

Although the operator splitting algorithms converge to the solution of the underlying problem as various discretization parameters tend to zero, it turns out that splitting approximations are too diffusive near self-sharpening fronts, at least when the splitting step Δt is large. We next present a numerical example that confirms this claim.

Example 4.1 (Operator Splitting). *This example is taken from Karlsen and Risebro [100]. We consider Burgers' equation; that is, $f(u) = \frac{1}{2}u^2$ and $d(u) = u$ in (65). This equation, introduced by Burgers [31] in 1940, represents a simplified model of the more complicated Navier-Stokes equations and captures some of the essential features of incompressible fluid dynamics; namely, a nonlinear convection term and a viscous diffusion term. The Burgers equation has a time independent solution given by*

$$(73) \quad u(x, t) = -\tanh\left(\frac{x}{2\varepsilon}\right),$$

so that it is well suited as a test case. The solution (73) corresponds to the case where the hyperbolic equation (67) would have a shock solution. We can also find an explicit solution in the case where the hyperbolic equation has a rarefaction wave solution, which corresponds to initial data of the form

$$(74) \quad u_0(x) = \begin{cases} -1, & \text{for } x \leq 0, \\ 1, & \text{for } x > 0. \end{cases}$$

By applying the Hopf-Cole transform, one finds that the solution is

$$u(x, t) = \frac{g(-x, t) - g(x, t)}{g(-x, t) + g(x, t)}, \quad g(x, t) = e^{\frac{t+x}{4\varepsilon}} \operatorname{erfc}\left(\frac{t+x}{\sqrt{4\varepsilon t}}\right).$$

In Figure 4, we show the operator splitting solutions at time $T = 1$ for both the "shock case" and the "rarefaction case". In this example, we use front tracking (see §5.2) to solve (67) and the Galerkin method (see §6.2) to solve (68). The most notable feature of these computations is the poor performance of the splitting algorithm in the shock case. The error turns out to be largely independent of the size of Δt in the rarefaction case, but it is very sensitive to the choice of Δt in the shock case. One should note that the error contribution in the shock case is due to the temporal splitting, and not the spatial discretization.

In view of Example 4.1, it can be tempting to conclude that operator splitting is a technique that is not particularly well suited to use with hyperbolic solvers that allow for large time steps. However, as we are about to learn, this is not the case! To better understand the (nonlinear) mechanisms behind the splitting error, one should bear in mind Oleĭnik's entropy condition, see Theorem 3.2. As we saw in Example 4.1, when Δt is larger than the diffusion scale ε , the standard splitting algorithm is too diffusive near the (self-sharpening) front. In view of Oleĭnik's theorem, this splitting error is simply a manifestation of the entropy condition being taken into account in the convection step. The entropy condition introduces a local convexification of $f(\cdot)$ representing the entropy loss associated with the shock in the hyperbolic solution. In other words, the operator splitting solution does not take into account the convex shape of the flux function, which in turn determines the self-sharpening nature of the (parabolic) front.

Luckily, the part of the flux function that is neglected (the entropy loss) can be identified as a residual flux term. For instance, assume that the solution of Burgers' equation is a moving steep

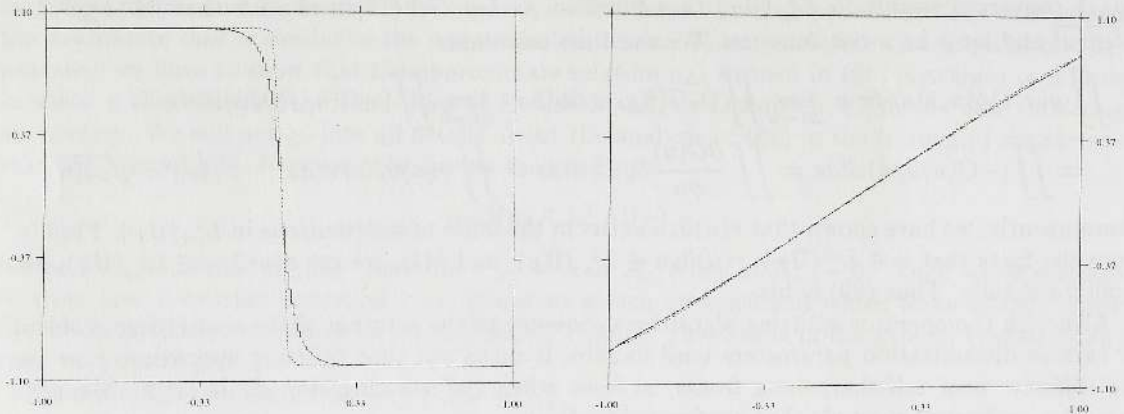


FIGURE 4. Exact solutions (dotted line) versus OS solutions (piecewise constant). The shock case (left) and the rarefaction case (right) are both calculated with $\Delta x = 0.01$, $\Delta t = 0.5$, and $\varepsilon = 0.01$. Observe that there is a significant amount of splitting error in the shock case due to the large time step.

front (as in Example 4.1) and that the hyperbolic solver produces a discontinuity with left and right limits v^l and v^r respectively. We can then identify the entropy loss associated with this shock as a residual flux term of the form

$$(75) \quad f_{\text{res}} = f - f_c.$$

Here, $f_c = f_c(v; v^l, v^r)$ denotes the correct envelope (dictated by the entropy condition) of f in the interval bounded by v^l and v^r , i.e.,

$$(76) \quad f_c(v; v^l, v^r) = \begin{cases} \text{the lower convex envelope of } f \text{ between } v^l \text{ and } v^r, & \text{if } v^l < v^r, \\ \text{the upper concave envelope of } f \text{ between } v^r \text{ and } v^l, & \text{if } v^l > v^r. \end{cases}$$

There are two ways to take the residual flux term f_{res} into account; that is, there are two ways to correct or counterbalance the splitting error. We can, for instance, perform a separate correction step after the diffusion step. Correction is then realized by solving the “residual” equation

$$(77) \quad \partial_t v + \partial_x f_{\text{res}}(v) = 0$$

over a time interval $(0, \tau)$, where $\tau > 0$ is some parameter that has to be chosen. Hence, instead of (66), we rely on an algorithm of the form (see Karlsen and Risebro [99])

$$(78) \quad u_{\Delta t}(x, n\Delta t) = [\mathcal{C}(\tau) \circ \mathcal{H}(\Delta t) \circ \mathcal{S}^f(\Delta t)]^n u_0(x), \quad \tau > 0,$$

where $\mathcal{C}(\tau)$ is the solution operator of (77), also called the correction operator. Note that when $\tau \equiv 0$, (78) reduces to the standard splitting defined in (66). The residual equation (77) represents the entropy loss generated in the convection step. The purpose of the correction step in (78) is to counterbalance the entropy loss so that the correct width of the self-sharpening front is ensured.

Another approach is to include the residual term in the equation modelling diffusion; that is, instead of solving the equation (68), we solve

$$(79) \quad \partial_t w + \partial_x f_{\text{res}}(w)_x = \varepsilon \partial_x (d(w) \partial_x w),$$

thereby yielding a splitting algorithm of the form (see Karlsen et al. [95])

$$(80) \quad u_{\Delta t}(x, n\Delta t) = [\mathcal{P}^{f_{\text{res}}}(\Delta t) \circ \mathcal{S}^f(\Delta t)]^n u_0(x),$$

where $\mathcal{P}^{f_{\text{res}}}(t)$ is the solution operator associated with (79). The point is that equation (79) contains the information needed to produce the correct width of the self-sharpening front. Since (80) does not involve the undetermined parameter τ that has to be “tuned”, algorithm (80) is the most important one for applications and is the one that we put foremost in these notes.

Note that the residual term f_{res} is “small”. In fact, following [99], it is not difficult to prove the estimate

$$\int |f_{\text{res}}(u_{\Delta t}(x, t_n))| dx = \mathcal{O}(\sqrt{\Delta t}),$$

where $u_{\Delta t}$ is defined in (78) or (80). Thus, (79) is much closer to being self adjoint than the original equation (65). This means that any iterative procedure will be more efficient for (79) than (65), and the numerical approximation properties will be better [10, 54]. Equation (79) may also be seen as an optimal upwind form of the original equation (65), where the amount of upwinding is determined by the mathematical model. Standard upwinding depends on the mesh size chosen for the problem, which may give severe grid orientation effects. A convection term determined by f_c in (75) gives a mass conserving upwinding and produces virtually no grid orientation effects [47]. It also produces a very good first approximation for (79). Within an iterative splitting strategy, the efficiency of the algorithm depends on the form chosen for f_c . A Riemann solver will give very accurate splittings because they provide “exact” information about the hyperbolic structure of the problem, see Example 4.2 below. Less accurate choices of f_c may give a simpler hyperbolic problem, but give a less efficient solution algorithm for the parabolic equation (79), see [80].

We have explained how to identify the entropy loss, i.e., the residual flux term, when the hyperbolic solution consists of a single shock wave. To describe the construction of a residual flux term in the general case, we assume that $f \in \text{Lip}_{\text{loc}}$ is piecewise linear with a finite number of breakpoints and that u^n is piecewise constant with a finite number of jumps. The reason for making these assumptions is that the exact solution $v(\cdot, t) = \mathcal{S}^f(t)u^n$ also will be piecewise constant with a finite number of jumps, see Theorem 5.1 in §5.2. Furthermore, the exact solution $v(\cdot, t)$ can be constructed by the front tracking method described in §5.2. In what follows, we suppress the time level dependency. The residual flux terms (associated with time level $t_n = n\Delta t$) can be constructed as follows: Observe that each jump in the solution $v(\cdot, t)$ is a shock obeying Oleinik’s entropy condition, (see Theorem 3.2). Suppose that the function $v(\cdot, t)$ is piecewise constant on a finite number of intervals with entropy satisfying discontinuities located at $\{x^k\}$. Let v^{k+1} denote the value of v in $[x^k, x^{k+1})$, and let $\{(y_1^k, y_2^k)\}$ be a sequence of pairs of spatial positions chosen so that $x^k \in (y_1^k, y_2^k)$ and $y_2^k \leq y_1^{k+1}$ for all k . Then we define the residual flux as

$$(81) \quad f_{\text{res}}(x, v) = \begin{cases} f(v) - f_c(v; k), & \text{for } x \in [y_1^k, y_2^k) \text{ and } v \in [v^k, v^{k+1}], \\ 0, & \text{for } x \in [y_1^k, y_2^k) \text{ and } v \notin [v^k, v^{k+1}], \end{cases}$$

where $f_c(v; k)$ denotes the correct envelope of f restricted to $[v^k, v^{k+1}]$, see (76). In an actual implementation, all shocks with strength below a certain threshold are disregarded, i.e., we switch off all residual fluxes for which $|v^k - v^{k+1}|$ is less than some (small) constant. Furthermore, we enlarge the spatial support of the nonzero residual fluxes, see Figure 5. Of course, equipped with the residual flux (81) we are free to choose either one of the corrected splitting algorithms defined in (78) and (80). We refer to [99] for further details about the residual flux.

The idea of using a residual flux term in the diffusion step was introduced by Espedal and Ewing [58], and further developed and analysed by Dahle, Espedal, and their collaborators [44, 45, 48, 46, 47] in the context of reservoir simulation. In many reservoir flow problems, the residual flux term may change on a very slow time scale compared with the convection scale. This may be true even for heterogeneous models [60]. This means that just a few of the parabolic corrections may be needed in a given time interval. This can give a far more efficient computer code if an efficient hyperbolic solver is available. For such fairly stable flow problems, a reasonable residual flux term can often be derived a priori by solving a single Riemann problem. For instance, to solve the convection-diffusion problem in Example 4.1 these authors would use an operator splitting algorithm in which the convection step is to solve the (almost linear) hyperbolic equation

$$(82) \quad \partial_t v + \partial_x f_c(v) = 0$$

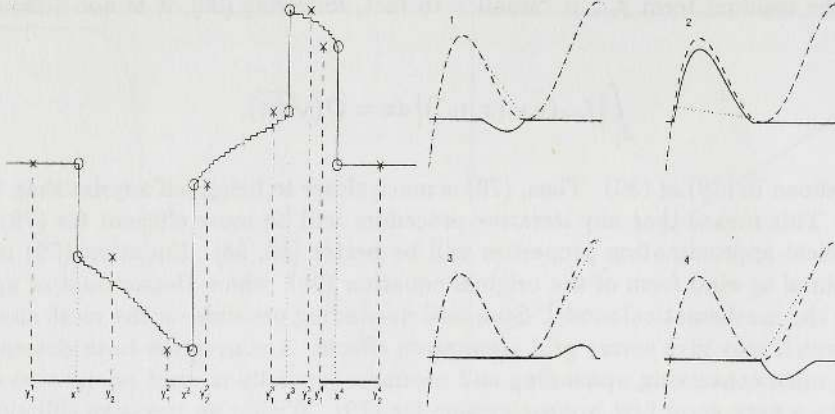


FIGURE 5. Left: Solution from a convection step where four shocks are identified in the spatial domain. Right: The corresponding residual flux functions: flux function (dash dotted), envelope function (dotted), and residual flux function (solid).

and the nonlinear diffusion equation (79), see Dahle [44] for further details. Using operator notation, their algorithm can be stated as

$$(83) \quad u_{\Delta t}(x, n\Delta t) = [\mathcal{P}^{f_{\text{res}}}(\Delta t) \circ \mathcal{S}^{f_c}(\Delta t)]^n u_0(x).$$

A fundamental difference between (83) and (80) is that (83) employs an a priori flux splitting; $f = f_c + f_{\text{res}}$, whereas (80) does not. The flux splitting is supposed be such that f_c represent most of the transport effects present in the original problem (65). If this is the case, then the modified method of characteristics [56] can be applied to (82) without severe time step restrictions, see §5.1 for further details. Moreover, the splitting algorithm defined in (83) has the advantage of giving the correct size of the shock layers, see Example 4.2 below. Following the method of proof that yielded Theorem 4.1, one can also show that the splitting algorithm defined in (83) converges to the solution of the underlying problem as $\Delta t \rightarrow 0$.

Of course, an a priori construction of a reasonable residual flux f_{res} is not possible for general problems, and new ideas were introduced by Karlsen and Risebro [99], and further developed and analysed by Karlsen et al. [95, 96, 98, 68, 22], which lead to the corrected operator algorithms defined in (78) and (80). To easily distinguish between the standard splitting algorithm defined in (66) and the more sophisticated splitting algorithms defined in (80) and (83), we refer to (66) as operator splitting (OS), whereas (80) and (83) are referred to as corrected operator splitting (COS) algorithms (we do not use (78) in these notes).

An extension of the corrected splitting algorithm defined in (80) to systems of convection-diffusion equations can be found in Natvig [123] and [49]. Concerning algorithm (83), we only point out that it is not as easily extendible to systems of equations as (80). This is due to the fact that it is not easy to produce a reasonable flux splitting for a system of equations.

We next present an example that demonstrates the corrected splitting algorithm defined in (83), and how one can derive a reasonable splitting of the convective flux f into two parts.

Example 4.2 (Corrected Operator Splitting/Flux Splitting). *We consider the convection-diffusion problem (65) with fluxes*

$$(84) \quad f(u) = \frac{u^3(1 - 10(1 - u)^3)}{u^3 + (1 - u)^3}, \quad d(u) = 4u(1 - u),$$

and Riemann initial data

$$u(x, 0) = \begin{cases} 0, & \text{for } x \leq 0.65, \\ 1, & \text{for } x > 0.65. \end{cases}$$

Note that the flux function $f(\cdot)$ is non-convex and that the diffusion function $d(\cdot)$ is nonlinear and has a two-point degeneracy; that is, $d(0) = d(1) = 0$. Consider a fluid in a one-dimensional

homogeneous porous medium consisting of two immiscible phases; a wetting phase, say, water and a non-wetting phase, say, oil. Let u denote the water saturation (and thus $1-u$ the oil saturation). Then the partial differential equation modelling the immiscible displacement of oil by water, under the influence of gravity, is of the form (65) with $f(\cdot)$ and $d(\cdot)$ given, e.g., as in (84).

To construct a convective flux splitting, we first note that the corresponding hyperbolic problem,

$$\partial_t v + \partial_x f(v) = 0, \quad v(x, 0) = \begin{cases} 0, & \text{for } x \leq 0.65, \\ 1, & \text{for } x > 0.65, \end{cases}$$

admits a travelling wave solution $v(x, t) = v(x/t)$ of the form

$$(85) \quad v\left(\frac{x}{t}\right) = \begin{cases} 0, & \text{for } \frac{x-0.65}{t} < f'_c(0), \\ (f'_c)^{-1}\left(\frac{x}{t}\right), & \text{for } \frac{x-0.65}{t} \in [f'_c(0), f'_c(1)], \\ 1, & \text{for } \frac{x-0.65}{t} > f'_c(1), \end{cases}$$

where f_c denotes the lower convex envelope of f restricted to the interval $[0, 1]$ and $(f'_c)^{-1}$ the inverse of its derivative. Having the piecewise smooth solution (85) in mind, we define the flux splitting by letting $f_{\text{res}} = f - f_c$; consult Figure 6 (left).

We are going to compare OS and COS solutions constructed by the algorithms defined in (66) and (83), respectively. In (83), we use the modified method of characteristics to solve (82) and the Petrov-Galerkin method to solve (79). In (66), we use front tracking (see §5.2) to solve (67) and finite differences (see §6.1) to solve (68). Solutions are computed up to time $T = 0.5$ and the scaling parameter ε is set to 0.01. In Figure 6 (middle) we show the OS calculation on the interval $[0, 2]$ using $\Delta x = 0.01$ and $\Delta t = 0.5$. In Figure 6 (right) we show the corresponding COS calculation. As was the case in Example 4.1, we see that OS produces too diffusive fronts when Δt is large. On the other hand, with the same Δt , we see that COS resolves the two fronts correctly.

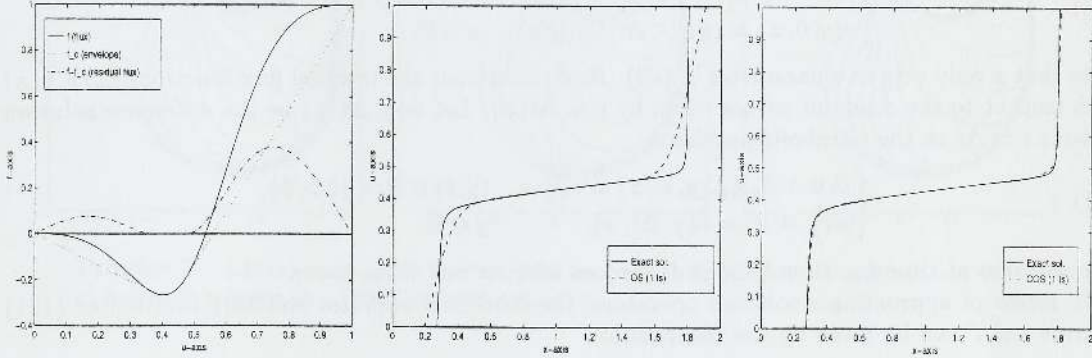


FIGURE 6. Left: The flux function (solid) and the flux splitting (dotted and dashdot). Middle: Exact solution versus OS using 1 time step and 200 mesh points. Middle: The exact solution versus COS using 1 time step and 200 mesh points. We see that COS' temporal splitting error is negligible compared with OS.

We now turn our attention to corrected operator splitting for multi-dimensional problems. Provided that one is equipped with a reasonable flux splitting, algorithm (83) remains the same for multi-dimensional problems, see §5.1 and §6.2 for further details. On the other hand, algorithm (80) is genuinely one-dimensional. But there are two obvious ways of generalising it to several space dimensions; namely, the method of streamlines or the method of dimensional splitting. Here we will rely on the latter approach. The streamline approach will be considered elsewhere.

For simplicity of notation, we only consider the two-dimensional problem

$$(86) \quad \begin{cases} \partial_t u + \partial_x f(u) + \partial_y g(u) = \varepsilon \Delta u, & (x, y, t) \in \mathbb{R}^2 \times (0, T), \\ u(x, y, 0) = u_0(x, y), & (x, y) \in \mathbb{R}^2. \end{cases}$$

The generalisation to higher dimensions (and more general diffusion functions) is straightforward. Consider a uniform Cartesian grid defined by the nodes $\{(i\Delta x, j\Delta y)\}$, where $\Delta x, \Delta y$ are given positive numbers and $i, j \in \mathbb{Z}$. Let π be the usual grid block averaging operator defined on this grid, that is,

$$(87) \quad \pi u(x, y) = \frac{1}{\Delta x \Delta y} \int_{z_{i,j}} u(\tilde{x}, \tilde{y}) d\tilde{x} d\tilde{y}, \quad \forall (x, y) \in z_{i,j},$$

where $z_{i,j}$ is grid block number (i, j) with lower left-hand corner in $(i\Delta x, j\Delta y)$. Let $f_\delta, g_\delta \in \text{Lip}_{\text{loc}}$ be piecewise linear approximations to f, g , respectively. Let u^n denote the fully discrete corrected splitting solution at some positive time $t = n\Delta t$, $u^0 = \pi u_0$. We next explain how to construct u^{n+1} from u^n . The idea is to use dimensional splitting coupled with the corrected operator splitting defined in (80) to solve one-dimensional equations.

x-sweep: Let $v(x, \Delta t; y)$ be the front tracking solution (see §5.2) at time $t = \Delta t$ to the hyperbolic problem

$$(88) \quad \begin{cases} \partial_t v + \partial_x f_\delta(v) = 0, & (x, t) \in \mathbb{R} \times \{t > 0\}, \\ v(x, 0; y) = u^n(x; y), & x \in \mathbb{R}. \end{cases}$$

Note that y only acts as a parameter in (88). Next, construct the residual flux function $f_{\text{res}}(x, v; y)$ with respect to the constant values taken by $v(x, \Delta t; y)$. Let $w(x, \Delta t; y)$ be the solution at time $t = \Delta t$ to the parabolic problem

$$(89) \quad \begin{cases} \partial_t w + \partial_x f_{\text{res}}(x, w; y) = \varepsilon \partial_x^2 w, & (x, t) \in \mathbb{R} \times \{t > 0\}, \\ w(x, 0; y) = v(x, \Delta t; y), & x \in \mathbb{R}, \end{cases}$$

computed using, e.g., an explicit or implicit central difference method (see §6.1).

y-sweep: Let $v(y, \Delta t; x)$ be the front tracking solution at time $t = \Delta t$ to the hyperbolic problem

$$(90) \quad \begin{cases} \partial_t v + \partial_y g_\delta(v) = 0, & (y, t) \in \mathbb{R} \times \{t > 0\}, \\ v(y, 0; x) = (\pi w(\cdot, \Delta t; \cdot))(y; x), & y \in \mathbb{R}. \end{cases}$$

Note that x only acts as a parameter in (90). Next, construct the residual flux function $g_{\text{res}}(y, v; x)$ with respect to the constant values taken by $v(y, \Delta t; x)$. Let $w(y, \Delta t; x)$ be the difference solution at time $t = \Delta t$ to the parabolic problem

$$(91) \quad \begin{cases} \partial_t w + \partial_y g_{\text{res}}(y, w; x) = \varepsilon \partial_y^2 w, & (y, t) \in \mathbb{R} \times \{t > 0\}, \\ w(y, 0; x) = v(y, \Delta t; x), & y \in \mathbb{R}. \end{cases}$$

The solution at time $t = (n+1)\Delta t$ is defined as $u^{n+1} = \pi w(\cdot, \Delta t; \cdot)$.

In terms of approximate solution operators, the corrected operator splitting solution of (101) at time $t = T$ can be given by the composition

$$(92) \quad u^N = \left[\mathcal{P}^{g_{\text{res}}, y}(\Delta t) \circ \mathcal{S}^{g_\delta, y}(\Delta t) \circ \mathcal{P}^{f_{\text{res}}, x}(\Delta t) \circ \mathcal{S}^{f_\delta, x}(\Delta t) \right]^N u^0,$$

where $\mathcal{P}^{g_{\text{res}}, y}$, $\mathcal{S}^{g_\delta, y}$, $\mathcal{P}^{f_{\text{res}}, x}$, and $\mathcal{S}^{f_\delta, x}$ denote the solution operators associated with the problems (91), (90), (89), and (88), respectively.

Remark 4.2. Observe that by ignoring the residual terms in the diffusion steps (89) and (91), the resulting standard operator splitting algorithm is slightly different than (53). It can also be shown that this algorithm converges to the solution of (86).

Remark 4.3. The stability result in Theorem 3.3 provides us with an estimate of the error contribution coming from the flux approximation used in (92). Let u and u_δ denote the solutions of the parabolic problem (86) with flux functions f, g and f_δ, g_δ , respectively. Suppose $f, g \in \text{Lip}_{\text{loc}}$ are piecewise C^2 , then the piecewise linear approximations f_δ, g_δ can be chosen so that

$$\|f - f_\delta\|_{\text{Lip}}, \|g - g_\delta\|_{\text{Lip}} = \mathcal{O}(\delta).$$

Consequently, using (30), we get

$$\|u(\cdot, t) - u_\delta(\cdot, t)\|_{L^1} = \mathcal{O}(\delta).$$

Example 4.3 (Corrected Operator Splitting). *This example is taken from Karlsen et al. [95]. Consider (86) with flux functions of the form*

$$f(u) = \frac{u^2}{u^2 + (1-u)^2}, \quad g(u) = f(u)(1 - 5(1-u)^2),$$

and initial data

$$u_0(x, y) = \begin{cases} 1, & \text{for } x^2 + y^2 < 0.5, \\ 0, & \text{otherwise.} \end{cases}$$

The solution is computed on the domain $[-1.5, 1.5] \times [-1.5, 1.5]$ up to time $T = 0.5$. We use $\delta = 0.01$ for the flux approximations. The reference solution is computed with OS (as defined in (92) with the residual fluxes set to zero) using a 1600×1600 grid and 441 time steps (CFL = 2.0). Figure 7 a) shows a contour plot of the solution obtained by OS using 5 time steps. The shock layer, but also the rarefaction area, is too wide. Note also the presence of a small artificial, almost vertical shock layer on the left-hand side of the peak. This is a result of the dimensional splitting, which is not able to completely resolve the dynamics of the problem. In Figure 7 b) we have used 10 time steps. The artificial shock layer has now (nearly) disappeared, and the resolution of the physical shock layers is slightly improved. Figure 8 a) shows the solution obtained by COS (as defined in (92)) using 5 time steps. The shock layer is of correct size, but as in Figure 7 a) the artificial shock layer is present. In Figure 8 b) the number of time steps has been doubled, and the solution is now in good correspondence with the reference solution.

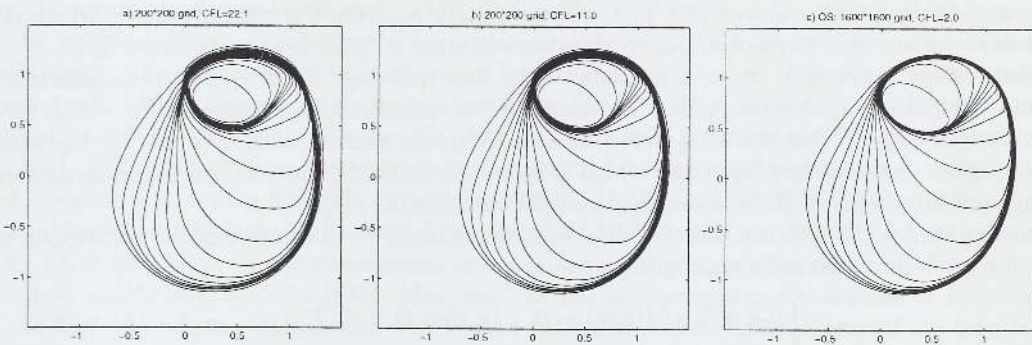


FIGURE 7. 2-D example. a) OS: 200×200 grid, CFL = 22.1. b) OS: 200×200 grid, CFL = 11.0. c) Reference solution on a 1600×1600 grid, CFL = 2.0.

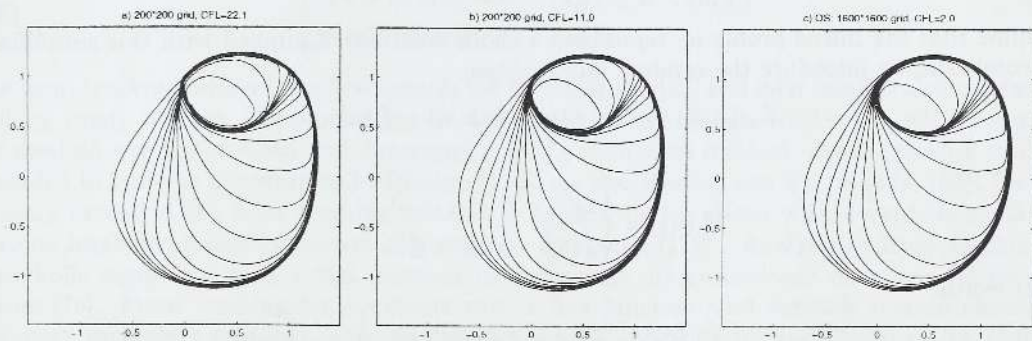


FIGURE 8. 2-D example. a) COS: 200×200 grid, CFL = 22.1. b) COS: 200×200 grid, CFL = 11.0. c) Reference solution on a 1600×1600 grid, CFL = 2.0.

5. HYPERBOLIC SOLVERS

Our numerical algorithms for solving the saturation equation (6) is based on splitting this convection-diffusion equation into a hyperbolic equation modelling convection and a (degenerate) parabolic equation modelling diffusion, see §4 for details. In the following we will describe two different methods for constructing the solution of the hyperbolic equation, see [79, 90, 105, 113, 146] for other alternatives. Numerical methods for the parabolic equation are presented in §6.

5.1. The Modified Method of Characteristics. The modified method of characteristics for linear convection-diffusion problems was introduced by Douglas and Russell [56]. This method was then extended to nonlinear problems by Espedal and Ewing [58]. To describe the modified method of characteristics [58], we consider the nonlinear convection-diffusion problem

$$(93) \quad \begin{cases} \partial_t u + \nabla \cdot F(x, u) = \varepsilon \nabla \cdot (d(x, u) \nabla u) + q(x), & (x, t) \in \Omega \times (0, T), \\ u(x, 0) = u_0(x), & x \in \Omega, \end{cases}$$

where $\Omega \subset \mathbb{R}^m$, $m = 1, 2, 3$, $q(x)$ is a source term, and the flux vector $F(x, u)$ is given as $f(u)v + f_g(u)K\nabla h$ (see §2). We assume that the initial function u_0 is monotonically decreasing from 1 to 0 in each space direction. The solution of (93) is supposed to satisfy the boundary condition

$$(94) \quad (F(x, u) - \varepsilon d(x, u) \nabla u) \cdot n = 0, \quad x \in \partial\Omega,$$

where n is the outer normal vector to $\partial\Omega$. In view of the operator splitting methodology described in §4, the idea is to use a flux splitting to separate out the transport part of (93). We then apply the modified method of characteristics to the transport problem and a Petrov-Galerkin method to the parabolic residual problem (see §6.2). The resulting solution algorithm for (93), which is a variant of the corrected operator splitting algorithm defined in (83), is demonstrated in §7.

We have some freedom in the construction of the flux splitting. To simplify the presentation, we assume that the gravity term $f_g(u)K\nabla h$ is completely included in the residual flux, which gives a uniform splitting. A flux splitting based on the complete flux function $F(x, u)$, on the other hand, will give a non-uniform splitting which is space dependent. The uniform and non-uniform splittings are discussed by Hansen and Espedal [80] and Frøysa [74].

Assuming that $f : \mathbb{R} \rightarrow \mathbb{R}$ is a S-shaped function, the entropy weak solution of the corresponding hyperbolic problem (with a decreasing u_0)

$$\begin{cases} \partial_t u + \nabla \cdot (f(u)v) = 0, & (x, t) \in \Omega \times (0, T), \\ u(x, 0) = u_0(x), & x \in \Omega, \end{cases}$$

develops a discontinuity with top shock value $u = u^s$ and bottom shock value $u = 0$. Consistent with the entropy condition, u^s may be determined by the Buckley-Leverett condition

$$s := \frac{f(u^s)}{u^s} = f'(u^s).$$

We assume that the initial profile u_0 represents a shock solution. Equipped with this simplified initial condition, we introduce the residual flux function

$$f_{\text{res}}(x, u) := b(x, u)u = F(x, u) - f_c(u)v,$$

where

$$f_c(u) := \begin{cases} su, & 0 \leq u < u^s, \\ f(u), & u^s \leq u \leq 1. \end{cases}$$

In other words,

$$(95) \quad f_{\text{res}}(x, u) = \begin{cases} (f(u) - su)v + f_g(u)K\nabla h, & 0 \leq u < u^s, \\ f_g(u)K\nabla h, & u^s \leq u \leq 1. \end{cases}$$

Let us divide the time interval $(0, T)$ into time slabs (t_{n-1}, t_n) , $n = 1, \dots, N$, where $t_0 = 0$, $t_N = T$, and $\Delta t = t_n - t_{n-1}$ is the time step. For $n = 1, \dots, N$, we will construct an approximate

solution u_h^n of (93) at time $t = t_n$. This will be done by a splitting procedure which alternates between solving a hyperbolic problem and parabolic residual problem. The hyperbolic problem is

$$(96) \quad \begin{cases} \partial_\tau u := \partial_t u + f'_c(u)v \cdot \nabla u = 0, & (x, t) \in \Omega \times (t_{n-1}, t_n), \\ u(x, 0) = u_h^{n-1}(x), & x \in \Omega, \end{cases}$$

where u_h^{n-1} is the approximate solution of (93) at the previous time level $t = t_{n-1}$, see §6.2. The residual problem is treated in §6.2. Integrating backwards along the characteristics, we get

$$(97) \quad \begin{cases} \bar{x} = x - \Delta t f'_c(\bar{u}^{n-1})v, \\ \bar{u}^{n-1} = u_h^{n-1}(\bar{x}), \end{cases}$$

The characteristic solution of (96) is unique and consists of a rarefaction wave and a shock wave. The integration can be made more accurate by using local time stepping within each global time slab (t_{n-1}, t_n) , see [70] for details. This is especially important for heterogeneous models.

Finally, the approximate solution u_h^n of (93) at time level $t = t_n$ is taken as the solution of the parabolic residual problem with initial data \bar{u}^{n-1} . This solution is constructed with a Petrov-Galerkin finite element method, see §6.2 for details.

It is well known that the characteristic procedure described above will give a small mass error. This error may be removed by introducing a ELLAM discretization. The Eulerian-Lagrangian localised adjoint method (ELLAM) of Celia et al. [33] is a general characteristic-based numerical solution procedure that applies to a variety of convection-diffusion type equations. In particular, ELLAM provides a consistent framework for treating general boundary conditions and maintaining mass conservation. Several authors [33, 136, 71, 73, 147, 154, 155] have developed ELLAM methods for the solution of one-dimensional linear equations with general inflow and outflow boundary conditions, while nonlinear equations are addressed by Dahle et al. [48]. The method has also been extended to problems containing reactive terms [34, 72]. The asymptotic convergence analysis and optimal-order error estimates for ELLAM methods have been obtained by Ewing and Wang [71, 155]. While all of these works have been restricted to one spatial dimension, some research have been carried out on multidimensional problems. Russell and Trujillo [137] and Binning [17] have addressed various issues in multidimensional ELLAM methods. Wang [152] has developed an ELLAM simulator to solve two-dimensional linear equations with general inflow and outflow boundary conditions, see also [153]. Moreover, he has also proved optimal-order error estimates for the ELLAM scheme and performed different numerical experiments. Some of the results have been reported in [71, 73].

5.2. Front Tracking Methods. We first describe a front tracking method for constructing approximate solutions to the one-dimensional hyperbolic problem

$$(98) \quad \begin{cases} \partial_t u + \partial_x f(u) = 0, & (x, t) \in \mathbb{R} \times (0, T), \\ u(x, 0) = u_0(x), & x \in \mathbb{R}. \end{cases}$$

The front tracking method was first introduced by Dafermos [42] and later used as a computational tool by many authors. In particular, Holden, Holden, and Høegh-Krohn [86, 85] proved that the method was well-defined and developed it into a numerical method. Front tracking was later extended to systems of equations by Risebro [132], see also Risebro and Tveito [133, 134]. Lie [115] recently extended the front tracking method to hyperbolic equations with a variable coefficient. Various implementation issues are discussed by Langseth [112]. Analysis of front tracking for hyperbolic equations with a flux function that depends discontinuously on u can be found in Gimse [76]. Front tracking for equations with a flux function that depends discontinuously on the space variable is analysed in Gimse and Risebro [77], Klingenberg and Risebro [103, 104], and Klausen and Risebro [102]. We refer to Holden and Risebro [90] for an excellent introduction to front tracking methods, see also Lie's thesis [116].

The front tracking method for (98) determines exact solutions within the class of step functions to a perturbed conservation law. For the moment, let us suppose that u_0 is piecewise constant and

f is continuous and piecewise linear with breakpoints at $\{u^0, \dots, u^N\}$. Observe that each jump in the initial data u_0 defines a Riemann problem; that is, (98) with data of the form

$$u_0(x) = \begin{cases} u^l, & x < 0, \\ u^r, & x > 0. \end{cases}$$

The solution of the Riemann problem generally consists of both rarefaction waves and shock waves. If the flux function is piecewise linear, the solution can be found by the technique outlined below.

Consider the Riemann problem with $u^l = u^0 \leq u^r = u^N$. Let f_c denote the lower convex envelope of f restricted to the interval $[u^l, u^r]$, see (76). Since f is piecewise linear then so is f_c . Let $\bar{u}^0 < \bar{u}^1 < \dots < \bar{u}^M$ be such that

$$\bar{u}^0 = u^0, \quad \bar{u}^M = u^N \quad \{\bar{u}^0, \dots, \bar{u}^M\} \subseteq \{u^0, \dots, u^N\},$$

and such that f_c is linear in each interval $[u^i, u^{i+1}]$. The solution of the Riemann problem with left state $u^l = u^0$ and right state $u^r = u^N$ is then given by

$$(99) \quad u(x, t) = \begin{cases} u^l, & x \leq \bar{s}^0 t \\ \bar{u}^i, & \bar{s}^i t < x \leq \bar{s}^{i+1} t, \quad i = 1, \dots, N-1, \\ u^r, & x > \bar{s}^{N-1} t, \end{cases}$$

where \bar{s}^i is the Rankine-Hugoniot shock speed,

$$\bar{s}^i = \frac{f_{i+1} - \bar{f}_i}{\bar{u}^{i+1} - \bar{u}^i} = f'_c(u^i), \quad i = 0, \dots, N-1,$$

and $\bar{f}_i = f(\bar{u}^i)$. When $u^l > u^r$ there is an similar formula involving the upper concave envelope. Note that since the flux function is piecewise linear, there are no rarefaction waves and each Riemann problem leads to a series of discontinuities propagating in the (x, t) - plane. The global solution of the perturbed problem (98) is obtained by connecting the solutions of the local Riemann problems defined by the piecewise constant initial data. This solution is well-defined until two or more discontinuities interact at some point. Then we have what is called a shock collision. A shock collision defines a new Riemann problem with left and right states given by the values immediately to the left and to the right of the colliding discontinuities. By solving this Riemann problem, the global solution is determined until the next shock collision occurs, and so on. We may continue in this fashion and thereby advance the (exact) solution up to any positive time. Holden, Holden, and Høegh-Krohn [86, 85] proved that this construction, which we call *front tracking*, is well-defined in the sense that there is a finite number of steps in the algorithm, even for infinite time. More precisely, the following theorem holds:

Theorem 5.1 ([86, 85, 90]). *Suppose that u_0 is a piecewise constant function with a finite number of discontinuities. Let $f \in \text{Lip}_{\text{loc}}$ be a piecewise linear function with a finite number of breakpoints. Then the problem (98) has an entropy weak solution $u(\cdot, t)$ which is piecewise constant for each fixed $t > 0$ and takes values in the set $\{u_0(x)\} \cup \{\text{the breakpoints of } f\}$. The solution $u(\cdot, t)$ can be constructed by front tracking in a finite number of steps for any $t > 0$.*

In the general case (arbitrary f and u_0), the front tracking method consists in replacing f by a suitable piecewise linear approximation $f_\delta \in \text{Lip}_{\text{loc}}$ and u_0 by a suitable piecewise constant approximation $u_{0, \Delta x}$. Here, $\delta > 0$ denotes the polygonal approximation parameter and Δx the spatial discretization parameter. Then this perturbed problem is solved according to the procedure outlined above. We denote the front tracking solution by u_Δ , where $\Delta = (\Delta x, \delta)$.

Remark 5.1. *Note that there is no time step (or CFL condition) associated with the front tracking method, and it introduces no artificial diffusion since a grid is only used to specify the initial data.*

Let us denote the front tracking solution by u_Δ , where $\Delta = (\delta, \Delta x)$. We have the following estimates:

$$(100) \quad \begin{cases} (a) & \|u_\Delta(\cdot, t)\|_{L^\infty} \leq \|u_0\|_{L^\infty}, \\ (b) & |u_\Delta(\cdot, t)|_{BV} \leq |u_0|_{BV}, \\ (c) & \|u_\Delta(\cdot, t_2) - u_\Delta(\cdot, t_1)\|_{L^1} \leq C|t_2 - t_1|. \end{cases}$$

Thanks to estimates (a)-(c) in (100), $\{u_\Delta\}$ is bounded in $BV(\mathcal{K})$ for any compact set $\mathcal{K} \subset \Pi_T$. Since BV is compactly imbedded into L^1 on compact sets, it is possible, after a diagonalization procedure, to produce a subsequence that converges in $L^1_{loc}(\Pi_T)$ to some limit u ,

$$u \in L^\infty(\Pi_T) \cap BV(\Pi_T).$$

Equipped with this strong convergence and the fact that each u_Δ is an entropy weak solution, it follows that the limit u is also an entropy weak solution. We can sum up as follows:

Theorem 5.2 ([42, 86, 85, 118]). *Suppose $u_0 \in L^1 \cap BV$ and $f \in \text{Lip}_{loc}$. Then the front tracking solution u_Δ converges in $L^1_{loc}(\Pi_T)$ to the unique entropy weak solution of (98) as $\Delta \rightarrow 0$. If, in addition, f is piecewise C^2 , then the following error estimate holds:*

$$\|u(\cdot, T) - u_\Delta(\cdot, T)\|_{L^1} \leq \text{Const} \cdot \Delta x + \text{Const}_T \cdot \delta.$$

The first part of this theorem is proved by Dafermos [42] and also Holden, Holden, and Høegh-Krohn [86, 85]. If one chooses f_δ and $u_{0, \Delta x}$ properly, the error estimate is a direct consequence of the general stability result found in Theorem 3.1.

Remark 5.2. *Using an approximation theorem of Tadmor [142], one can obtain an improved error estimate for the front tracking method. To this end, we must restrict ourselves to Lip^+ bounded initial data u_0 and a strictly convex flux function f . We then have (see [94] for a proof)*

$$\|u(\cdot, T) - u_\Delta(\cdot, T)\|_{W^{-1,1}} \leq \text{Const} \cdot \Delta x^2 + \text{Const}_T \cdot \delta^2.$$

Recall that the norm $\|w(x, t)\|_{W^{-1,1}}$ can be defined when $\int w(x, t) dx = 0$ as

$$\|w(x, t)\|_{W^{-1,1}} = \left\| \int_{-\infty}^x w(\xi, t) d\xi \right\|_{L^1}.$$

One should note that front tracking is second order accurate in the weak $W^{-1,1}$ norm. This fact is in contrast to most difference methods, which are typically first order accurate in this norm.

The front tracking method for a hyperbolic equation with a variable coefficient, i.e., $\partial_x f(u)$ in (98) is replaced by $v(x)\partial_x f(u)$ for some smooth function $v(x)$, is more or less the same. The only difference is that the discontinuity lines $x(t)$ in the (x, t) plane are no longer straight lines, but given as solutions of the differential equation $x'(t) = v(x)s$, where s is the Rankine-Hugoniot shock speed $s = f_\delta(u^l) - f_\delta(u^r)/(u^l - u^r)$. By approximating the velocity $v(x)$ by a piecewise constant or piecewise linear function, the differential equation can be solved explicitly and the discontinuity lines $x(t)$ given in closed form, we refer to Lie [115] for details.

Holden and Risebro [89] proposed to extend the front tracking method to multi-dimensional equations by the means of dimensional splitting. For simplicity we consider the two-dimensional case. A generalisation to higher dimensions is straightforward. Let us start with the semi-discrete dimensional splitting method. Consider the two-dimensional hyperbolic problem

$$(101) \quad \begin{cases} \partial_t u + \partial_x f(u) + \partial_y g(u) = 0, & (x, y, t) \in \Pi_T = \mathbb{R}^2 \times (0, T), \\ u(x, y, 0) = u_0(x, y), & (x, y) \in \mathbb{R}^2, \end{cases}$$

whose entropy weak solution is denoted by $u(t) = \mathcal{S}(t)u_0$. Let $v(t) = \mathcal{S}^{f,x}(t)v_0$ and $w(t) = \mathcal{S}^{g,y}(t)w_0$ denote the entropy weak solutions of the one-dimensional problems

$$\begin{aligned} \partial_t v + \partial_x f(v) &= 0, & v|_{t=0} &= v_0, \\ \partial_t w + \partial_y g(w) &= 0, & w|_{t=0} &= w_0. \end{aligned}$$

Then the semi-discrete dimensional splitting solution is defined as

$$(102) \quad S(n\Delta t)u_0 \approx [S^{g,y}(\Delta t) \circ S^{f,x}(\Delta t)]^n u_0.$$

The semi-discrete algorithm (102) was proved to be convergent by Crandall and Majda [40] using a compactness argument. A convergence rate estimate for (102) was later proved independently by Teng [145] and Karlsen [93] using Kuznetsov's approximation theory [110].

In applications, we replace the exact solutions operator by front tracking. More precisely, consider a uniform Cartesian grid defined by the nodes $\{(i\Delta x, j\Delta y)\}$, where $\Delta x, \Delta y$ are given positive numbers and $i, j \in \mathbb{Z}$. Let π be the usual grid block averaging operator defined on this grid, see (87). Furthermore, let f_δ and g_δ be piecewise linear approximations to f and g , respectively, and $S^{f_\delta,x}(t)$ and $S^{g_\delta,y}(t)$ the corresponding one-dimensional solution operators. Then the fully discrete dimensional splitting solution at time $t = t_n$ is defined as

$$(103) \quad u_\Delta(x, y, t_n) = [\pi \circ S^{g_\delta,y}(\Delta t) \circ \pi \circ S^{f_\delta,x}(\Delta t)]^n \pi u_0,$$

where $\Delta = (\Delta x, \Delta y, \Delta t, \delta)$. The dimensional splitting method (103) consists in using front tracking in the x -direction for a small time step Δt . Note that the front tracking solution will not necessarily be piecewise constant on the original grid. The solution is therefore projected back onto this grid before we apply front tracking in the y -direction for a time step Δt , using the (projected) solution computed in the x -direction as initial data, and so on.

Remark 5.3. *It should be noted that no CFL condition is associated with the numerical method (103). Multi-dimensional computations using CFL numbers as high as 10 – 20 (with satisfactory results) have been reported, see Lie, Haugse, and Karlsen [117]. Computational results for multi-dimensional systems of equations can be found in Holden, Lie, and Risebro [88] for the Euler equations and Holdahl, Holden, and Lie [84] for the shallow water equations.*

With $u^n = u_\Delta(t_n)$, we introduce the short-hand notations

$$u^{n+1/2} = \pi \circ S^{f_\delta,x}(\Delta t)u^n, \quad u^{n+1} = \pi \circ S^{g_\delta,y}(\Delta t)u^{n+1/2}.$$

Note that we have only defined $u_{\Delta t}$ at the discrete times t_n . In between two consecutive discrete times, we use the following time interpolant:

$$(104) \quad u_\Delta(x, y, t) = \begin{cases} S^{f_\delta,x}(2(t - t_n))u^n, & t \in (t_n, t_{n+1/2}), \\ u^{n+1/2}, & t = t_{n+1/2}, \\ S^{g_\delta,y}(2(t - t_{n+1/2}))u^{n+1/2}, & t \in (t_{n+1/2}, t_{n+1}), \\ u^{n+1}, & t = t_{n+1}. \end{cases}$$

We have the following convergence results for (104):

Theorem 5.3 ([89, 93]). *Suppose $u_0 \in L^1 \cap L^\infty \cap BV$ and $f, g \in \text{Lip}_{\text{loc}}$. Then the fully discrete dimensional splitting solution u_Δ converges in $L^1_{\text{loc}}(\Pi_T)$ to the unique entropy weak solution of (101) as $\Delta \rightarrow 0$. If, in addition, f, g are piecewise C^2 , then the following error estimate holds:*

$$\|u(\cdot, T) - u_\Delta(\cdot, T)\|_{L^1} \leq \text{Const}_T \cdot (\sqrt{\Delta t} + \sqrt{\Delta x} + \delta).$$

The first part of this theorem was proved by Holden and Risebro [89]. The error estimate is due to Karlsen [93], see also Lie, Haugse, and Karlsen [117]. We refer to Lie [114] for the details concerning the extension of the dimensional splitting method (103) to equations with variable coefficients (velocity fields). Finally, we mention that a reservoir simulator based on front tracking methods is described in [19, 20].

6. PARABOLIC SOLVERS

To solve convection-diffusion problems we use the operator splitting algorithms described in §4. However, as we thoroughly explained in §4, it may become necessary to employ a correction strategy (or a suitable flux splitting) to reduce the splitting error when the time step is large. Hence the diffusion part of an operator splitting is not merely to solve a pure diffusion equation,

but an equation containing both convection and diffusion terms. We thus need parabolic solvers that are capable of solving general convection-diffusion equations.

Below we describe some finite difference methods and a Petrov-Galerkin finite element method. The Petrov-Galerkin method is capable of solving convection-diffusion equations which may degenerate at some isolated points, and is thus well suited for the reservoir simulation problems we have in mind (see §2). The finite difference methods are capable of solving both degenerate and strongly degenerate convection-diffusion equations. Consequently, operator splitting algorithms based on finite differences for the parabolic updates can also be applied to mathematical models containing strongly degenerate parabolic equations, see [27, 28].

6.1. Finite Difference Methods. Let us first consider the one-dimensional, possibly strongly degenerate, convection-diffusion problem

$$(105) \quad \begin{cases} \partial_t u + \partial_x f(u) = \partial_x (d(u) \partial_x u), & (x, t) \in \Pi_T = \mathbb{R} \times (0, T), \\ u(x, 0) = u_0(x), & x \in \mathbb{R}, \end{cases}$$

where $f, d \geq 0, u_0$ are given, sufficiently regular functions. As we mentioned in §3, solutions of (105) can become discontinuous in finite time. For a given initial condition a plenitude of weak solutions may exist. Consequently, we need a selection mechanism — an entropy condition — to single out the physical interesting weak solution, see §3 and Definition 3.3 for details. Evje and Karlsen [64, 65, 67] have recently developed a convergence theory for a class of finite difference methods for problems such as (105). This theory, which, roughly speaking, states that any consistent, conservative-form, monotone difference method converges to the physically correct solution of (105), can be viewed as an direct extension of the classical monotone difference theory developed by Harten, Hyman, and Lax [81] and Crandall and Majda [41] for conservation laws.

Selecting a mesh size $\Delta x > 0$, a time step $\Delta t > 0$, and an integer N so that $N\Delta t = T$, the value of our difference approximation at $(x, t) = (j\Delta x, n\Delta t)$ will be denoted by u_j^n . To simplify the notation, we introduce the difference operators

$$\Delta_- u_j = \frac{1}{\Delta x} (u_j - u_{j-1}), \quad \Delta_+ u_j = \frac{1}{\Delta x} (u_{j+1} - u_j).$$

We consider consistent, conservative, monotone, $(2p+1)$ -point finite-difference methods of the form

$$(106) \quad \frac{u_j^{n+1} - u_j^n}{\Delta t} + \Delta_- (F(u^n; j) - \Delta_+ D(u_j^n)) = 0,$$

where $D(u)$ is defined in (26) and $F(u^n; j) = F(u_{j-p+1}^n, \dots, u_{j+p}^n)$ is the numerical flux associated with the convection part of (105). The initial data for (106) is taken as

$$u_j^0 = \frac{1}{\Delta x} \int_{j\Delta x}^{(j+1)\Delta x} u_0(x) dx.$$

To make the methods (106) consistent with the convection-diffusion equation (105) it is sufficient to require that

$$F(u, \dots, u) = f(u).$$

The assumption of monotonicity guarantees that (106), when viewed as an algorithm of the form

$$u_j^{n+1} = \mathcal{S}(u_{j-p+1}^n, \dots, u_{j+p}^n) =: \mathcal{S}(u^n; j),$$

has the property that \mathcal{S} is a non-decreasing function of all its arguments.

Let us give an example of a three-point ($p=1$) monotone scheme. For a monotone flux f , the upwind scheme is defined by

$$(107) \quad F(u_j^n, u_{j+1}^n) = \begin{cases} f(u_j^n), & \text{if } f' > 0, \\ f(u_{j+1}^n), & \text{if } f' < 0. \end{cases}$$

More generally, for a non-monotone flux f , the generalised upwind scheme of Engquist and Osher is defined by

$$F(u_j^n, u_{j+1}^n) = f^+(u_j^n) + f^-(u_{j+1}^n),$$

where

$$f^+(u) = f(0) + \int_0^u \max(f'(s), 0) ds, \quad f^-(u) = \int_0^u \min(f'(s), 0) ds.$$

A simple calculation reveals that the upwind method and the generalised upwind method both are monotone methods provided the following CFL type condition holds:

$$(108) \quad \max |f'| \frac{\Delta t}{\Delta x} + 2 \max |d| \frac{\Delta t}{\Delta x^2} \leq 1.$$

Let u_Δ , $\Delta = (\Delta x, \Delta t)$, be the interpolant of degree one associated with the discrete data points $\{u_j^n\}$; that is, u_Δ interpolates at the vertices of each rectangle $R_j^n = [j\Delta x, (j+1)\Delta x] \times [n\Delta t, (n+1)\Delta t]$. Note that u_Δ is continuous everywhere and differentiable almost everywhere. Regarding the sequence $\{u_\Delta\}$, we have the following main convergence theorem:

Theorem 6.1 ([65]). *The sequence $\{u_\Delta\}$ built from (106) converges in $L^1_{loc}(\Pi_T)$ to the unique generalised solution (in the sense of Definition 3.3) of (105) as $\Delta \rightarrow 0$. Furthermore, $\{D(u_\Delta)\}$ converges uniformly on compact sets $\mathcal{K} \subset \Pi_T$ to $D(u) \in C^{1, \frac{1}{2}}(\bar{\Pi}_T)$ as $\Delta \rightarrow 0$.*

Here, $C^{1, \frac{1}{2}}(\bar{\Pi}_T)$ denotes the space of functions that are Hölder continuous with exponent 1 in the space variable and 1/2 in the time variable. An important part of the proof of this theorem is to establish the following three estimates for $\{u_j^n\}$:

- $$\left\{ \begin{array}{l} \text{(a) a uniform } L^\infty \text{ bound,} \\ \text{(b) a uniform total variation bound,} \\ \text{(c) } L^1 \text{ Lipschitz continuity in the time variable,} \end{array} \right.$$

and the following two estimates for the discrete total flux $F(u^n; j) - \Delta_+ D(u_j^n)$:

- $$\left\{ \begin{array}{l} \text{(d) a uniform } L^\infty \text{ bound,} \\ \text{(e) a uniform total variation bound,} \end{array} \right.$$

see [65] for details. Then, using the three estimates (a)-(c), it is not difficult to show that there is a finite constant $C = C(T) > 0$ (independent of Δ) such that

$$\|u_\Delta\|_{L^\infty(\Pi_T)} + |u_\Delta|_{BV(\Pi_T)} \leq C.$$

Hence, the sequence $\{u_\Delta\}$ is bounded in $BV(\mathcal{K})$ for any compact set $\mathcal{K} \subset \Pi_T$. Since $BV(\mathcal{K})$ is compactly imbedded into $L^1(\mathcal{K})$, it is possible to select a subsequence that converges in $L^1(\mathcal{K})$. Furthermore, using a standard diagonal process, we can construct a sequence that converges in $L^1_{loc}(\Pi_T)$ to a limit u ,

$$u \in L^\infty(\Pi_T) \cap BV(\Pi_T).$$

For notational simplicity, let $w_\Delta = D(u_\Delta)$. It is possible to use estimates (d) and (e) to prove that w_Δ satisfies the following Hölder estimate (see [65]):

$$|w_\Delta(y, \tau) - w_\Delta(x, t)| \leq C \left(|y - x| + \sqrt{|\tau - t|} + \Delta x + \sqrt{\Delta t} \right),$$

where $C > 0$ is a finite constant not depending on Δ, x, y, t, τ . By repeating the proof of the Ascoli-Arzelà compactness theorem, we deduce the existence of a subsequence of $\{w_\Delta\}$ converging uniformly on each compactum $\mathcal{K} \subset \Pi_T$ to a limit w ,

$$w \in C^{1, \frac{1}{2}}(\bar{\Pi}_T).$$

Let $\{\Delta_j\}$ be a sequence of discretization parameters tending to zero such that $u_{\Delta_j} \rightarrow u$ a.e. and $w_{\Delta_j} \rightarrow w$ uniformly on compacta as $j \rightarrow \infty$ (such a sequence can certainly be found). Since u_{Δ_j} converges to u a.e. and w is continuous, we conclude that

$$w = D(u).$$

Finally, convergence of $\{u_{\Delta}\}$ to the correct physical solution of (105) follows from the cell entropy inequality ($k \in \mathbb{K}$)

$$\frac{|u_j^{n+1} - k| - |u_j^n - k|}{\Delta t} + \Delta_- (F(u^n \vee k; j) - F(u^n \wedge k; j) - \Delta_+ |D(u_j^n) - D(k)|) \leq 0,$$

where $u \vee v = \max(u, v)$ and $u \wedge v = \min(u, v)$. This discrete entropy inequality is in turn an easy consequence of the monotonicity of \mathcal{S} . The reader is referred to [65] for further details on the convergence analysis.

Remark 6.1. *In many applications it is desirable to avoid the explicit stability restriction (108). One way to overcome (108) is of course to use an implicit version of (106). By combining the arguments in [65] with the Crandall and Liggett theory [39], it is possible to analyse implicit methods as well, see [67] for details.*

It is also possible to speed up explicit methods by using a so-called super time stepping procedure. Super time stepping (STS) is a simple and effective method that speeds up explicit methods for parabolic equations, rendering them as useful as any implicit method, while retaining its simplicity and better accuracy, see Alexiades et al. [4, 5] for details. In [68], the STS method has been used (with good results) as a part of our operator splitting methodology.

Remark 6.2. *A formally second order (in space) version of (106) can be obtained via a MUSCL type approach, which is by now a classical approach in the context of conservation laws. It uses a piecewise linear reconstruction, instead of piecewise constant, together with a limitation procedure, see Evje and Karlsen [63] for analytical and numerical results.*

Remark 6.3. *The finite difference theory can be generalised to doubly nonlinear degenerate parabolic equations of the form (48), see Evje and Karlsen [64] for details.*

A novel feature of our difference methods (106) is that they are based on differencing the conservative-form equation

$$\partial_t u + \partial_x (f(u) - \partial_x D(u)) = 0,$$

and not the equation in its original form. Of course, one can devise methods based on differencing (105) directly, yielding, for example, methods of the form

$$(109) \quad \frac{u_j^{n+1} - u_j^n}{\Delta t} + \Delta_- (F(u^n; j) - d(u_{j+1/2}^n) \Delta_+ u_j^n) = 0,$$

where $u_{j+1/2}^n = \frac{1}{2}(u_j^n + u_{j+1}^n)$. Indeed, the diffusion discretization in (109) is commonly used in the case of uniformly parabolic equations, see, e.g., [122]. Although it is possible to prove that the non-conservative method (109) converges to a limit, this limit does not seem to satisfy the entropy condition; that is, the method (109) does not seem to converge to the physically correct solution of (105) in the case of strong degeneracy. The following numerical example demonstrates this.

Example 6.1 (Non-Conservative Methods). *This example is taken from Evje and Karlsen [65]. We consider (105) with fluxes*

$$\tilde{f}(u) = \frac{1}{4}u^2, \quad \tilde{d}(u) = 4d(u),$$

where $d(\cdot)$ is given in (47). We have computed solutions with (106) and (109) using very fine discretization parameters. In these calculations the upwind flux (107) was used in (106) and (109). The computed solutions are shown in Figure 9. Clearly, the non-conservative method (109) produces a **wrong** solution. Moreover, the difference between this solution and the (correct!) solution produced by (106) seems to increase with time. We are currently investigating this phenomenon.

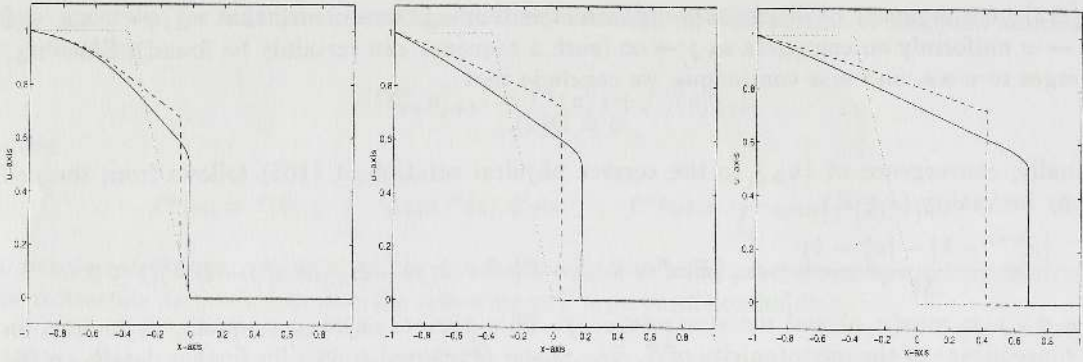


FIGURE 9. Plots of solutions produced by the difference methods defined in (106) (solid) and (109) (dashed) at three different times; $T = 0.0625$ (left), $T = 0.25$ (middle), and $T = 1.0$ (right). The initial function is shown as dotted.

See Hou and LeFloch [91] for an analysis of difference methods for hyperbolic equations which use a non-conservative discretization of the flux function.

Finally, let us very briefly discuss the multi-dimensional case. For simplicity of notation, we consider only the two-dimensional problem

$$(110) \quad \begin{cases} \partial_t u + \partial_x f(u) + \partial_y g(u) = \partial_x (d(u) \partial_x u) + \partial_y (d(u) \partial_y u), \\ u(x, y, 0) = u_0(x, y). \end{cases}$$

Let $u_{j,k}^n$ denote the finite difference approximation at $(x, y, t) = (j\Delta x, k\Delta y, n\Delta t)$. A conservative finite difference method for (110) takes the form

$$(111) \quad \frac{u_{j,k}^{n+1} - u_{j,k}^n}{\Delta t} + \Delta_{x,-} (F(u^n; j, k) - \Delta_{x,+} D(u_{j,k}^n)) + \Delta_{y,-} (G(u^n; j, k) - \Delta_{y,+} D(u_{j,k}^n)) = 0,$$

where $\Delta_{\ell,-}$, $\Delta_{\ell,+}$ are the backward and forward differences, respectively, in direction ℓ , for $\ell = x, y$, and F, G are convective numerical fluxes that are consistent with f, g , respectively. The initial data for (111) is taken as

$$u_{j,k}^0 = \frac{1}{\Delta x \Delta y} \int_{z_{j,k}} u_0(x, y) dx dy, \\ z_{j,k} = (i\Delta x, (i+1)\Delta x) \times (j\Delta y, (j+1)\Delta y).$$

For further details on multi-dimensional monotone difference methods and partial convergence results, we refer to [65]. Finally, we mention that the difference methods described in this section apply equally well to equations with variable coefficients.

6.2. A Petrov-Galerkin Method. In this section we describe a Petrov-Galerkin method for solving the parabolic residual problem resulting from the splitting algorithm described in §5.1. We refer to Morton [122] for a detailed introduction to Petrov-Galerkin methods. For $n = 1, \dots, N$, the parabolic residual problem takes the form

$$(112) \quad \begin{cases} \partial_t u + \nabla \cdot (b(x, u)u - d(x, u)\nabla u) = \bar{q}(x, t), & (x, t) \in \Omega \times (t_{n-1}, t_n), \\ u(x, t_{n-1}) = \bar{u}^{n-1}(x), & x \in \Omega, \end{cases}$$

where the residual fractional flow function $f_{\text{res}}(x, u) = b(x, u)u$ is defined in (95), $\bar{q}(x, t)$ is a source term, the initial condition $\bar{u}^{n-1}(x)$ is given in (97), and the time slab (t_{n-1}, t_n) is defined in §5.1. We note that with this definition of f_{res} , the numerical solution of (93) automatically satisfies the boundary condition (94) where $v(x) \cdot n = 0$.

Using the characteristic solution of (96) to approximate the time derivative and to linearise the nonlinear coefficients in (112), the Petrov-Galerkin method will introduce a symmetrization

of (112), see [10, 92]. Let $H^1(\Omega)$ denote the usual Sobolev space formed by all functions in $L^2(\Omega)$ whose gradients belong to $L^2(\Omega)$. Let $H_0^1(\Omega)$ and V be subsets of $H^1(\Omega)$ such that [10, 44]

$$H_0^1 := \left\{ w \in H^1(\Omega) : w(x) = 0 \text{ for } x \in \partial\Omega \right\},$$

$$V := \left\{ w \in H^1(\Omega) : w \text{ satisfies the given boundary conditions} \right\}.$$

We now obtain the following weak formulation of (112): Find $u \in V$ such that

$$(113) \quad \begin{cases} (\partial_t u, w) + B(u, w) = (\tilde{q}(x, t_{n-1}), w), & t \in (t_{n-1}, t_n), \forall w \in H_0^1. \\ u(x, t_{n-1}) = \bar{u}^{n-1}(x), & x \in \Omega, \end{cases}$$

where the bilinear form $B(\cdot, \cdot)$ is defined as

$$(114) \quad B(u, w) = (\nabla \cdot (b(x, u)u), w) + \varepsilon(d(x, u)\nabla u, \nabla w)$$

and (\cdot, \cdot) denotes the usual $L^2(\Omega)$ inner product. To deduce (113) from (112) we have used integration by parts. The boundary terms arising from this partial integration are included in the right-hand side $(\tilde{q}(x, t_{n-1}), w)$ of (113). Note that the boundary terms will in general depend nonlinearly on the unknown. We use, however, the characteristic solution \bar{u}^{n-1} to linearise the boundary terms. One should also note that the the boundary condition for (112) will depend on the chosen flux splitting, see [74, 75, 80] for further details.

Equipped with the characteristic solution \bar{u}^{n-1} of (96), we can replace the parabolic problem (113) by the following linearised elliptic problem: For $n = 1, \dots, N$, find $u^n \in V$ such that

$$(115) \quad (u^n, w) + \Delta t B(u^n, w) = (\bar{u}^{n-1}, w) + (\tilde{q}(x, t_{n-1}), w), \quad \forall w \in H_0^1,$$

where the time step Δt has been introduced in §5.1. As a first step in an iterative procedure [80], the nonlinear coefficients are linearised as

$$b(x) := b(x, \bar{u}^{n-1}) \quad \text{and} \quad d(x) := d(x, \bar{u}^{n-1}).$$

With the components of $d(x)$ in $C^0(\bar{\Omega})$ and $b(x) \in H^1(\Omega)$, $B(\cdot, \cdot)$ defines a bilinear continuous form on $H_0^1 \times H_0^1$. Unfortunately, the sign of $B(\cdot, \cdot)$ is indefinite due to the transport term. However, we have [44, 47]

$$|\Delta t (\nabla \cdot (b(x)w), w)| < (w, w) + \varepsilon \Delta t (d(x)w, w),$$

which means that the complete bilinear form $A(\cdot, \cdot)$, where

$$A(u, w) = (u, w) + \Delta t B(u, w),$$

is coercive on $H^1(\Omega) \times H^1(\Omega)$. Hence the Lax-Milgram theorem ensures the existence of a unique element u^n satisfying the elliptic problem (115). In the following we restrict the presentation to $\Omega \subset \mathbb{R}^2$. The trial and optimal test spaces used within the Petrov-Galerkin formulation are given as follows: Let $\{x_{i,j}\}$ be the nodes generating a rectangular mesh covering Ω . We then introduce a trial space $S^h \subset H^1(\Omega)$ spanned by the trial functions $\{\theta_{i,j}\}$ and a test space $T^h \subset H^1(\Omega)$ spanned by the test functions $\{\psi_{i,j}\}$, where h denotes the grid spacing. Furthermore, we introduce the discrete subspaces

$$S_0^h = S^h \cap H_0^1, \quad T_0^h = T^h \cap H_0^1, \quad S_V^h = S^h \cap V.$$

Then the Petrov-Galerkin finite element formulation of (115) reads as follows: For $n = 1, \dots, N$, find $u_n^n \in S_V^h$ such that

$$(116) \quad A(u_n^n, \psi) = (\bar{u}^{n-1}, \psi) + (\tilde{q}(x, t_{n-1}), \psi), \quad \forall \psi \in T_0^h.$$

It is well known that using $T^h = S^h$ (as in the usual Galerkin formulation) is a bad choice of test space when the transport term $b(x)$ dominates the diffusion term. This appears as unphysical oscillations in the numerical solution in the presence of a steep front. It may also be demonstrated that this problem is caused by the dominating transport term in the discretized bilinear form $B(\cdot, \cdot)$, i.e., the leading part of $A(\cdot, \cdot)$ in the steep front region. To handle such problems, Barrett and Morten [10] have developed a symmetrization technique in one space dimension that yields optimal approximation properties in suitable norms. The symmetrization technique used in one

space dimension is in principle easily extendible to several space dimensions, but the extension may be technically involved and produces test functions that are difficult to use in practical computations. A procedure that resolves this problem has been developed by Demkowicz and Oden [54], who introduce the concept of "numerical optimal" test functions. Here, we use tensor products of one-dimensional test functions to define optimal test functions in several space dimensions.

Approximate optimal test functions in one space dimension, which yield an almost symmetric bilinear form when measured in a suitable norm [10, 82, 92], take the form

$$(117) \quad \psi_i(x) = \begin{cases} 0, & x < x_{i-1}, \\ \theta_i(x) + c_i \sigma_i(x), & x_{i-1} \leq x \leq x_i, \\ \theta_i(x) + c_i \sigma_i(x), & x_i < x \leq x_{i+1}, \\ 0, & x > x_{i+1}, \end{cases}$$

where

$$c_i = 3 \left(\frac{2}{\beta_i} - \coth \left(\frac{\beta_i}{2} \right) \right), \quad \beta_i = \frac{b(x_i)h}{\varepsilon d(x_i)}.$$

In (117), $\theta_i(x)$ is the hat function

$$\theta_i(x) = \begin{cases} 0, & x < x_{i-1}, \\ \frac{x - x_{i-1}}{h}, & x_{i-1} \leq x \leq x_i, \\ \frac{x_{i+1} - x}{h}, & x_i < x \leq x_{i+1}, \\ 0, & x > x_{i+1}, \end{cases}$$

and $\sigma_i(x)$ is the quadratic perturbation

$$\sigma_i(x) = \begin{cases} \frac{(x - x_{i-1})(x - x_i)}{h^2}, & x_{i-1} \leq x \leq x_i, \\ -\frac{(x - x_i)(x - x_{i+1})}{h^2}, & x_i < x \leq x_{i+1}. \end{cases}$$

The test functions are depicted in Figure 10. The test functions in two dimensions are defined as

$$\psi_{i,j}(x, y) = \psi_i(x)\psi_j(y),$$

where $\psi_i(x)$ and $\psi_j(y)$ are defined above, see, e.g., [44] for further details.

As noted earlier, the porous media flow models may give solutions which vary on a wide range of scales in space and time. A proper resolution of the flow at wells, moving fronts, and the dynamics caused by large permeability variations at fractures and faults will require a very fine mesh. Such phenomena may be fairly local, separated by regions of slow variation. Thus, both the pressure-velocity equations and the Petrov-Galerkin formulation of the flow equation can represent very large elliptic problems. If a uniform mesh adequate for the fine scale variation is chosen, the problem may simply be too big for any computer. Therefore, an adaptive local grid refinement solution procedure is needed in order to reduce the problem to a solvable size. This can be achieved by using a preconditioned iterative solution procedure based on domain decomposition methods [140]. We will give the main steps in such a solution procedure for the flow equation (116), see [129, 47, 143] for further details. Assuming that we are given a coarse grid Ω_C on the computational domain Ω , we get the following algorithm:

1. Solve the hyperbolic problem (96) on the coarse grid Ω_C using the modified method of characteristics.
2. Identify coarse elements where the error is too large. This may be done simply by selecting elements which contain large gradients in the solution or by using an error estimator. Then activate refined overlapping/non overlapping sub grids Ω_k to each of these.
3. Solve (96) on the refined sub grids Ω_k .
4. Solve (116) on the refined coarse elements using domain decomposition methods. The characteristic solution of (96) is used as the boundary conditions for the sub domains Ω_k . Using an overlapping domain decomposition method will reduce the error introduced by the choice of boundary conditions, see [129, 143]

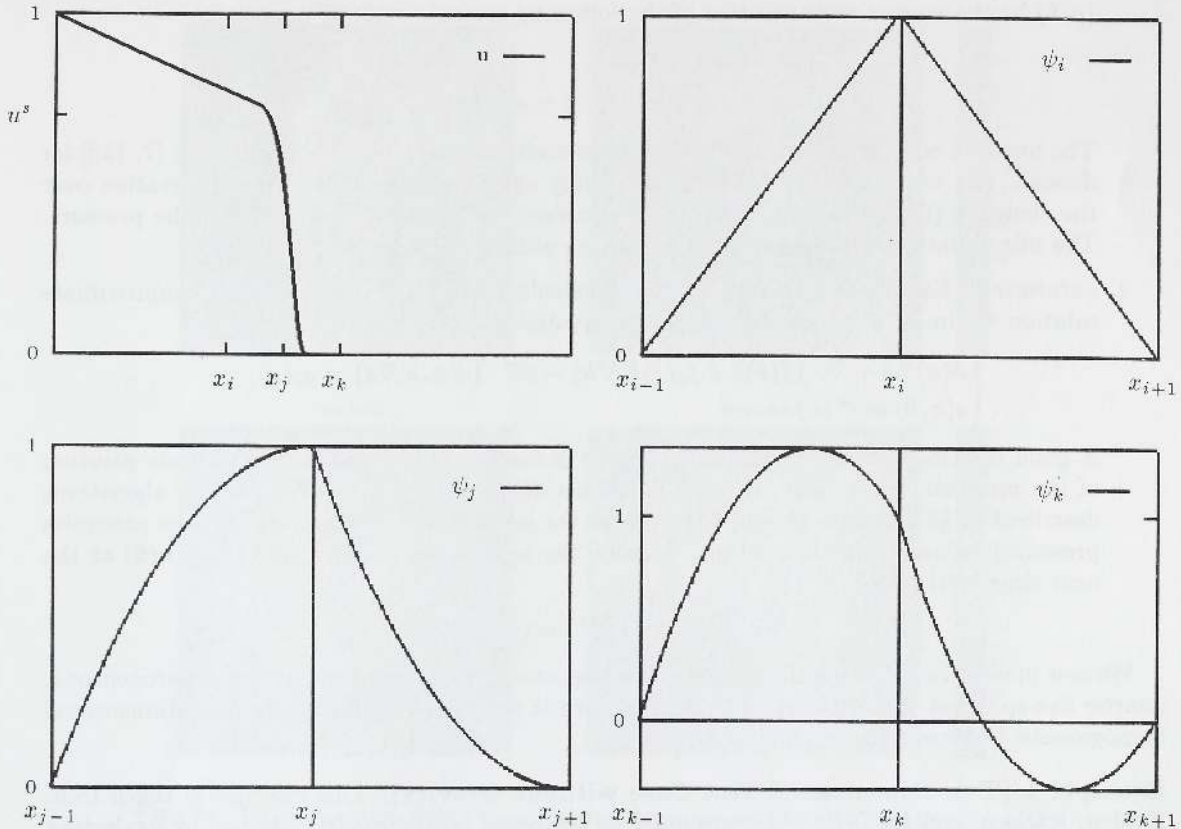


FIGURE 10. Typical test functions for the convection-diffusion problem (93). Upper left plot: A typical one-dimensional solution profile. The corresponding test functions are shown in the following three plots. Upper right plot: Test function for $u > u^s$. Lower left plot: Test function for $0 < u < u^s$. Lower right plot: Test function for $u = 0$.

It is well known that numerical algorithms based on domain decomposition methods have good parallel properties [140], which means that large complex problems may be solved [46].

Remark 6.4. *It is an open problem to prove L^1 convergence of an operator splitting algorithm based on, e.g., the modified method of characteristic and the Petrov-Galerkin method.*

7. RESERVOIR SIMULATION

We now apply the numerical algorithms developed in the previous sections to the reservoir flow model (4)-(5)-(6). The governing equations (4)-(5)-(6) constitute a coupled system of nonlinear partial differential equations. A sequential time stepping procedure is used to decouple the equations, which essentially consists of solving one equation at the time, starting with the pressure equation to generate a velocity field. Subsequently, this velocity field is used as input in the saturation equation, and so on. This strategy reflects the different nature of the elliptic pressure equation and the convection dominated parabolic saturation equation. For an analysis of this time stepping procedure we refer the reader to Kruřkov and Sukorjanskiĭ [106].

Let T_s be the final computing time, and choose a sequential time step Δt_s , and an integer $N_s \geq 1$ such that $N_s \Delta t_s = T_s$. Let the (p^n, v^n, s^n) denote the approximate solution of the reservoir flow model (4)-(5)-(6) at time $t = n \Delta t_s$, for some $n = 0, \dots, N_s - 1$. The approximate solution at the next time level is computed in the following two steps:

1. *Pressure:* Since the velocity field is smoother than the saturation field, we use the saturation field from the previous time level to linearise the pressure-velocity equations (4)-(5). Let

(\bar{p}, \bar{v}) be the approximate solution of the following pressure-velocity equations:

$$\begin{cases} \nabla \cdot v = q_1(x), \\ v = -K(x)\lambda(s^n)(\nabla \bar{p} - \rho(s^n)\nabla h). \end{cases}$$

The pressure equation is solved by a Galerkin method with bilinear elements, see [7, 138] for details. The velocity is derived from the Darcy equation using local flux conservation over the elements [138], which gives the same accuracy for the velocity field as for the pressure. The mixed finite element method would be an alternative solution procedure.

2. *Saturation*: Equipped with the velocity \bar{v} calculated in Step 1, let \bar{s} be the approximate solution at time $t = \Delta t_s$ of the saturation equation

$$\begin{cases} \phi(x)\partial_t \bar{s} + \nabla \cdot (f(\bar{s})\bar{v} + f_g(\bar{s})K\nabla h) - \varepsilon \nabla \cdot (d(x, s)\nabla \bar{s}) = q_2(x), \\ s(x, 0) = s^n(x). \end{cases}$$

A good treatment of the saturation equation is essential for obtaining an accurate solution of the reservoir flow model (4)-(5)-(6). We use the corrected operator splitting algorithms described in §4 (see also §5 and §6) to solve the saturation equation, see the two examples presented below for further details. Finally, the approximate solution of (4)-(5)-(6) at the next time level is defined by

$$(p^{n+1}, v^{n+1}, s^{n+1}) = (\bar{p}, \bar{v}, \bar{s}).$$

We now present two numerical examples. The first example is a two-dimensional, heterogeneous, quarter five-spot test case without a gravity term, while the second example is a three-dimensional homogeneous test case with a gravity term.

Example 1 (Two-Dimensional Test Case without Gravity). This example is taken from Holden, Karlsen, and Lie [87]. The computations are based on the model obtained by neglecting the gravity term in equations (4)-(5)-(6). To simulate this model, we use the corrected splitting algorithm defined in (92) based on front tracking (see §5.2) for the convection updates and finite differences (see §6.1) for the diffusion updates. Similar simulations are presented in Espedal and Langlo [60] using the algorithm defined in (83). These authors use the modified method of characteristics (see §5.1) for the convection updates and the Petrov-Galerkin method (see §6.2) for the diffusion updates.

The permeability field (see Figure 11) is generated as $K(x) = \exp(Z(x))$, where $Z(x)$ is a Gaussian field. Figure 12 shows saturation fields computed for viscosity ratios $\mu_o : \mu_w$ equal 1:1 and 5:1. The diffusion coefficient is $\varepsilon = 0.01$, the simulation grid has 129×129 blocks, and we use $N_s = 20$ sequential time steps to reach final time $T_s = 0.8$ with a CFL number 2.0 for the saturation solver (up to water breakthrough).

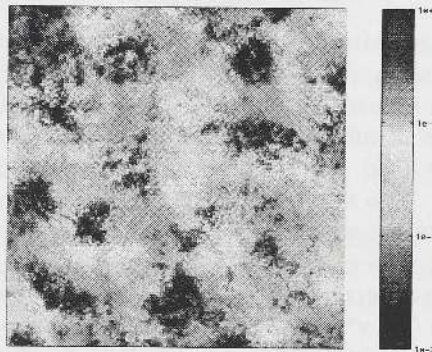


FIGURE 11. Permeability field plotted on a logarithmic colour scale.

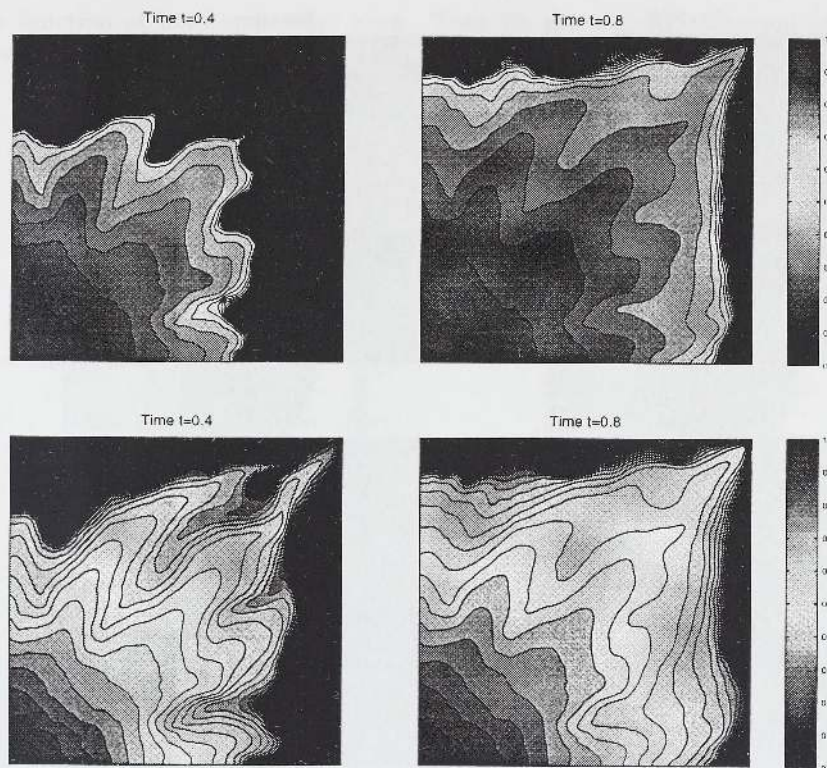


FIGURE 12. Saturation fields from quarter five-spot simulations for viscosity ratios $\mu_o : \mu_w$ equal 1:1 (top) and 5:1 (bottom).

Next, we consider a permeability field containing low-permeable blocks which are barriers to the flow (see Figure 13). Figure 14 shows the saturation fields computed for viscosity ratios $\mu_o : \mu_w$ equal 20:1 and 1:2. The diffusion coefficient is $\varepsilon = 0.01$ and we use a 257×257 grid with 80 sequential time steps to reach final time 0.8 and CFL number 2.0 in the saturation solver. As for the above case, the fingering effects are more pronounced at the adverse viscosity ratio. Notice also the improved areal sweep and penetration into low-permeable regions in the lower plot. Fine scale solutions such as those presented in this example are very accurate. Consequently, they can be used good reference solutions for upscaling problems, see, e.g., [59, 60, 83].

We refer to [87] for further details about the computations presented in this example.

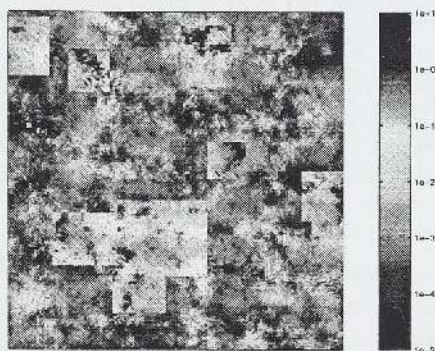


FIGURE 13. Permeability field with low-permeable regions plotted on a logarithmic colour scale.

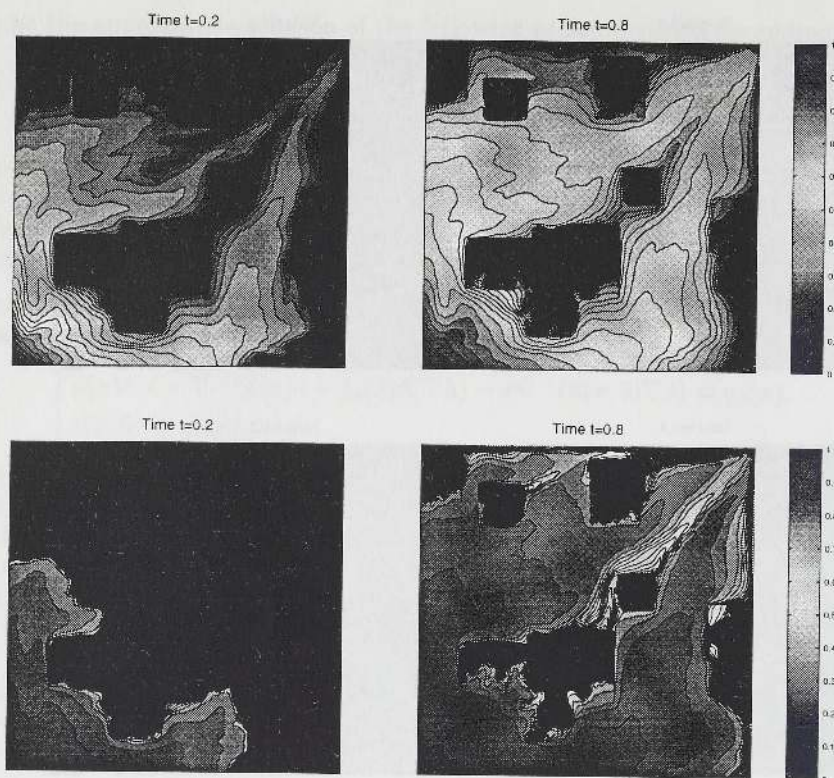


FIGURE 14. Saturation fields from quarter five-spot simulations (with low-permeable regions) for viscosity ratios $\mu_o : \mu_w$ equal 20:1 (top) and 1:2 (bottom).

Example 2 (Three-Dimensional Test Case with Gravity). This example is taken from Frøysa and Espedal [75], see also Frøysa [74]. The computations are based on the model described by equations (4)-(5)-(6). To simulate this model, we use the corrected splitting algorithm defined in (83) based on the modified method of characteristics (see §5.1) for the convection updates and the Petrov-Galerkin finite element method (see §6.2) for the diffusion updates. A flux splitting which is uniform in space has been applied (see §5.1), but local node based splittings have also been tested, see [75]. We use the following dimensionless data:

$$\left\{ \begin{array}{ll} \Omega & = [0, 1] \times [0, 1] \times [0, 0.5]. \\ \text{Grid} & = 21 \times 21 \times 15. \\ \text{Rates} & = 0.04 \text{ in injector, } -0.04 \text{ in producer.} \\ \text{Gravity} & = g \nabla h = [0, 0, -g]. \\ \text{Time step} & = 0.01. \\ \text{Initial profile} & = \begin{cases} \text{if } (x + y) \leq 0.5 \\ \quad \text{if } z \geq 0.2 \\ \quad \quad s = 1.0 - (x + y) \\ \quad \text{else} \\ \quad \quad s = 5z(1.0 - (x + y)) \\ \text{else} \\ \quad s = 0. \end{cases} \end{array} \right.$$

The injection well is a line well located on the z -axis with $z \in [0.25, 0.5]$. A similar vertical production well is located at position $(x, y) = (1, 1)$ with $z \in [0, 0.25]$. In the test case, the z component of the velocity field mostly has the same sign as the gravity. The initial saturation gradient $\partial_z s$, however, is positive but changes sign as the saturation front moves along. The sign

change is a function of both space and time. Thus we get a good indication of how well the methods handle a saturation field that "turns".

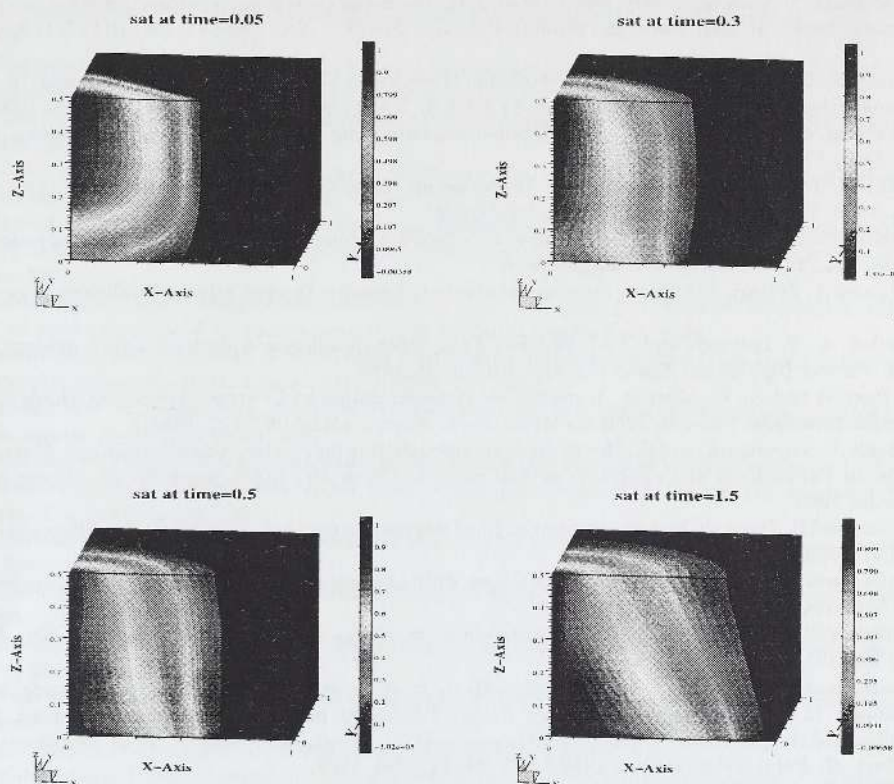


FIGURE 15. The saturation field at times $t = 0.05$, $t = 0.3$, $t = 0.5$, and $t = 1.5$

Figure 15 shows the saturation field with the uniform flux splitting described in §5.1. Similar results are obtained with a non-uniform splitting, see [74, 75]. After a few time steps the water has reached the bottom boundary and the saturation gradient $\partial_z s$ starts to change sign. At $t = 0.05$, there are regions with $\partial_z s < 0$ and regions with $\partial_z s > 0$, but no oscillations are visible. At $t = 0.3$, the gradient $\partial_z s$ is negative everywhere, except for a region in the vicinity of the injector. The present example gives a fairly difficult boundary condition, but the tests shows that the diffusion step in the solution algorithm handles these accurately. The results also indicate that the numerical algorithms are able to handle a "turning" field without introducing oscillations.

We refer to [75, 74] for further details about the computations presented in this example.

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