Fraunhofer ITWM

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Berichte des Fraunhofer ITWM, Nr. 206 (2011)

ISSN 1434-9973

Bericht 206 (2011)

Die Veröffentlichungen in der Berichtsreihe des Fraunhofer ITWM können bezogen werden über:

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Vorwort

Das Tätigkeitsfeld des Fraunhofer-Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe werden sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen.

Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

A One-Dimensional Model of the Pressing Section of a Paper Machine Including Dynamic Capillary Effects

O. Iliev · G. Printsypar · S. Rief

Abstract This work presents the dynamic capillary pressure model (Hassanizadeh, Gray, 1990, 1993a) adapted for the needs of paper manufacturing process simulations. The dynamic capillary pressure-saturation relation is included in a one-dimensional simulation model for the pressing section of a paper machine. The one-dimensional model is derived from a two-dimensional model by averaging with respect to the vertical direction. Then, the model is discretized by the finite volume method and solved by Newton's method.

The numerical experiments are carried out for parameters typical for the paper layer. The dynamic capillary pressure-saturation relation shows significant influence on the distribution of water pressure. The behaviour of the solution agrees with laboratory experiments (Beck, 1983).

Keywords steady modified Richards' equation · finite volume method · dynamic capillary pressure · pressing section of a paper machine

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1 Introduction

Paper plays an important role in our everyday life. Manufactures all over the world produce millions of tons of paper every year. People use more then 5,000 products which are made from paper. From the industrial point of view, papermaking is a complicated and expensive industrial process. This challenging problem attracts attention of many scientists, who investigate and simulate the papermaking process.

The paper machine typically consists of four main sections (see, e.g. Metso Corporation (2010)): the head box, the forming section, the pressing section and the drying section. The head box provides the suspension which consists of 99% water and 1% fibers. Typically the forming section is a continuous rotating wire mesh that removes water from the paper suspension at first by natural gravity filtration and then with the help of co-called suction boxes. The dry solids content of the suspension increases to about 20% after this section. The third section of the paper machine is the pressing section. It provides the dewatering of the paper layer by mechanical pressing of a sandwich of the paper layer and a properly selected felt. The simplest press nip consists of two rotating rolls with layers of paper and felts transported at high speed between them (see Figure 1). The felt is a special highly porous clothing which provides void space, so that during the pressing, the water is squeezed out of the paper and enters the felt. The dry solids content in the paper is about 50%-55% after the pressing section. The last section of a papermaking machine is the drying section, where the water which still remains in the paper layer, is removed by evaporation, as the sheet is held in close contact to large heated cylinders. The drying is very expensive, therefore understanding and improving the dewatering in the pressing section is highly demanded by the industry, and attracts increasing attention from researchers.

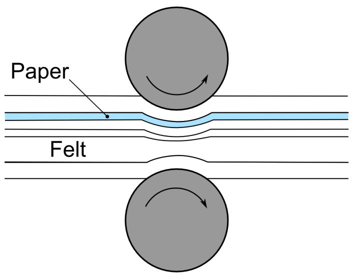

Fig. 1 The simplest construction of the pressing nips

We are concerned with the modeling and the simulation of the pressing section. There exist different approaches to model this problem. Most of the models consider three phase flow (solid, water and air) (Bezanovic et al., 2006, 2007a,b; Hiltunen, 1995; Kataja et al., 1992). The problem is very complex, therefore there is no unique description, and different models are used in these works. In Hiltunen (1995); Kataja et al. (1992) the conservation of mass and momentum is used together with a Lagrangian formulation along displacement characteristic lines (solid flow lines). In Bezanovic et al. (2006, 2007a,b) the mass balance equations in Lagrangian formulation are used. Moreover, Bezanovic et al. (2007b) considers the compressible air case. But all these models have a common feature, which is neglecting the capillary forces. Models which take into account the capillary effect are presented in Bermond (1997); Rief (2005); Velten et al. (2000). The model described by Bermond (1997) uses a two-phase flow model including capillary pressure-saturation relation and introduces thermal aspects. In Rief (2005); Velten et al. (2000) the Richards approach for flow in unsaturated porous media is adopted. As a starting point we have chosen the 1D model realized in Velten et al. (2000).

The capillary pressure is often of critical importance in modeling flow in porous media (see e.g. Bear, Bachmat, 1990). The classical approach (Bear, Bachmat, 1990) for dealing with capillary effects provides the definition of macroscopic capillary pressure as a difference between average pressures of nonwetting and wetting phases and quantifies:

$$p_n - p_w \equiv p_c = f(S).$$

A large number of scientists have worked on understanding and parametrization of this functional relation, mainly in connection with soil. Among those studies, the most famous are the models of air-water systems by Leverett (1941), Broocks, Corey (1964) and Van Genuchten (1980). The relationships they derived have been validated for certain flow regimes and types of porous media in numerous experiments. However, many experimental results show that these relationship are satisfied only under equilibrium conditions (see Hassanizadeh et al. (2002) and references therein). Thus, each point on a drainage or imbibition capillary pressure-saturation curve is measured after increasing pressure by one step, and waiting until equilibrium is reached. The time to equilibrium after each step ranges from a few hours to many days. Hence, the construction of the complete curve takes weeks. And consequently, the capillary pressure-saturation relation which is obtained under these conditions can not accurately describe filtration processes which involve rapid changes of the saturation.

To resolve this issue, new approaches have appeared recently. Theoretical studies were performed by Barenblatt et al. (1987, 2002), Kalaydjian (1992), Bourgeat, Panfilov (1998) and Hassanizadeh, Gray (1990, 1993a) to appraise the dynamic effect in the capillary pressure, which can not be captured by existing empirical relations. Here we have chosen to work with the model introduced by Hassanizadeh and Gray, having in mind that it was derived taking into account physical aspects of the filtration process. It was possible to adapt this model to the specific features of our problem.

The first goal of this paper is to adapt the dynamic capillary pressure model of Hassanizadeh, Gray (1990, 1993a) for the needs of the paper manufacturing process simulations. Then the second objective is to present an extension of the 1D model in Velten et al. (2000) for processes in the pressing section of the papermaking machine, by accounting for the dynamic effects in the capillary pressure-saturation relation. Note, that in the above mentioned papers denoted to dynamic effects in the capillary pressure-saturation relation, the latter are accounted via including terms with time-derivative of the saturation. For the papermaking machine, we end up with a model including a space derivative of the saturation. This is due to the fact that the paper-felt sandwich is transported with about 1500-2000 m/min between the roles, and follows from the full model derived by Hassanizadeh, Gray (1990, 1993a). For fixed porous media the term with the space derivative of the saturation vanishes. We are not aware of any other paper where the dynamical effects are accounted by the space derivative of the saturation.

In short, the objectives of this paper are to present an accurate one-dimensional model and to study the influence of the dynamic capillary pressure-saturation relation on the solution of the problem describing the pressing section of a paper machine. The mathematical model, which describes the basic physical principles behind the pressing process, is developed in Section 2. In Section 3, the discretization by finite volumes is presented. The implementation of the Newton-iteration method for the discrete problem is discussed in Section 4. Section 5 presents the numerical results. Finally, we draw conclusions in Section 6.

2 Mathematical model

2.1 Modeling two-dimensional flow

Concerning the modeling of the pressing section of a paper machine, the porous media is composed of three phases: solid (denoted by index "s"), liquid (or water) (index "w") and air (index "a"). An *Eulerian approach* is used to describe our system. The computational domain $\Omega \subset \mathbb{R}^2$ and its boundary Γ ($\overline{\Omega} = \Omega \cup \Gamma$) are shown in Figure 2. Let $f_l(x)$ and $f_u(x)$ be the functions which describe the lower and upper profiles of the paper-felt sandwich, respectively. Then $\overline{\Omega} = \{(x, z) : x \in [A, B], z \in [f_l(x), f_u(x)]\}$, where boundaries $x = A$ and $x = B$ are fixed points far away from the press rolls and $A < B$.

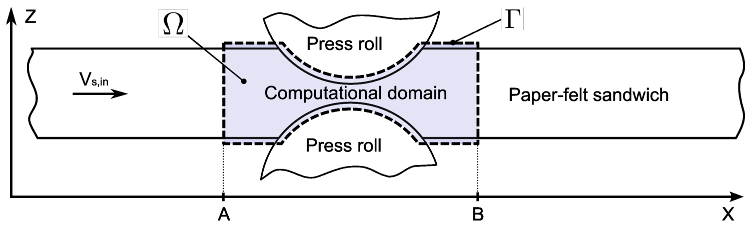

Fig. 2 Location of roll press nip and computational domain

As indicated in Figure 2, let us assume that the paper-felt sandwich is transported through the press nips from the left to the right with velocity $V_{s,in}$ measured in $[m/s]$. The horizontal direction is designated as x-direction, while z-direction is the vertical component. The third direction is neglected since the length of the cylindrical roll is large, and side boundary effects are not considered.

The general form of the mass conservation equation in *Eulerian form* (Bear, 1972; Bear, Verruijt, 1987; Helmig, 1997) for each phase α, without sources and sinks, is:

$$\frac{\partial \rho_\alpha^*}{\partial t}(\mathbf{x}, t) + \operatorname{div}(\rho_\alpha^* \mathbf{V}_\alpha)(\mathbf{x}, t) = 0, \ \alpha = s, w, a, \ \mathbf{x} = (x, z) \in \Omega, t \in \mathbb{R}_+, \tag{1}$$

where t is the time in $[s]$, $\mathbf{V}_\alpha$ denotes the velocity of phase α in $[m/s]$, ρ_α^* is the volume fraction of phase α in $[kg/m^3]$. The solid velocity denoted as $\mathbf{V}_s$ appears as a result of the transportation and deformation processes. Let us also remark that in the following all vectors and tensors will be marked with bold type.

Let S ($[-]$) be the dimensionless saturation of the liquid phase, ϕ ($[-]$) be the porosity and ρ_α be the density of phase α, which is measured in $[kg/m^3]$. Then:

$$\rho_s^* = (1-\phi)\rho_s, \tag{2}$$
$$\rho_w^* = \phi S \rho_w, \tag{3}$$
$$\rho_a^* = \phi(1-S)\rho_a. \tag{4}$$

By inserting equations (2)-(4) into equation (1), we obtain:

for the solid:
$$\frac{\partial((1-\phi)\rho_s)}{\partial t} + \operatorname{div}((1-\phi)\rho_s \mathbf{V}_s) = 0, \tag{5}$$

for the liquid:
$$\frac{\partial(\phi S \rho_w)}{\partial t} + \operatorname{div}(\phi S \rho_w \mathbf{V}_w) = 0, \tag{6}$$

for the air:
$$\frac{\partial(\phi(1-S)\rho_a)}{\partial t} + \operatorname{div}(\phi(1-S)\rho_a \mathbf{V}_a) = 0. \tag{7}$$

From now on, we assume that the air is at atmospheric pressure. This assumption, in connection with paper dewatering, was earlier successfully employed in Rief (2005); Velten et al. (2000). Therefore, the air pressure is known and saturation of the air phase can be computed as $S_a = 1 - S$. Thus, only two mass conservation equations for the solid and for the water (5), (6) are considered.

To define water and solid velocities, $\mathbf{V}_w$, $\mathbf{V}_s$, in addition to the mass conservation equations we have to consider momentum conservation. The momentum equation for water phase can be represented by a generalized Darcy's law. We neglect gravity and take into account the solid velocity:

$$\phi S(\mathbf{V}_w - \mathbf{V}_s) = -\frac{k_{rw}}{\mu_w}\mathbf{K}\operatorname{grad} p_w, \tag{8}$$

where k_{rw} ($[-]$) is the relative permeability of the water phase, μ_w is the viscosity of water in $[Pa \cdot s]$, $\mathbf{K}$ is the intrinsic permeability tensor in $[m^2]$, p_w is the water pressure in $[Pa]$.

Momentum conservation for the solid phase yields (Bear, 1972; Bear, Bachmat, 1990):

$$\rho_s^* \frac{D^s\mathbf{V}_s}{Dt} - \operatorname{div}\mathbf{t}_s = \sum_{(\alpha)} \rho_\alpha^* \mathbf{F}_\alpha \quad \text{or} \quad (1-\phi)\rho_s \frac{D^s\mathbf{V}_s}{Dt} - \operatorname{div}\mathbf{t}_s = \sum_{(\alpha)} \rho_\alpha^* \mathbf{F}_\alpha, \tag{9}$$

where $\mathbf{t}_s$ is the second-rank symmetrical stress tensor measured in $[Pa]$, $\mathbf{F}_\alpha$ is the external force per unit mass of phase α acting on particles of this phase in $[m/s^2]$, $\frac{D^s\mathbf{V}_s}{Dt}$ is the material derivative, which takes the form:

$$\frac{D^s\mathbf{V}_s}{Dt} = \frac{\partial \mathbf{V}_s}{\partial t} + (\mathbf{V}_s \cdot \operatorname{grad})\,\mathbf{V}_s. \tag{10}$$

We assume that the liquid and solid phases are incompressible ($\rho_s = const$, $\rho_w = const$), however, the porous media gets deformed (via rearrangement of the solid skeleton). Hence, porosity is a function of space and time $\phi = \phi(\mathbf{x}, t)$.

Thereby, the mass conservation equations yield for the solid phase:

$$-\frac{\partial \phi}{\partial t} + \operatorname{div}((1-\phi)\mathbf{V}_s) = 0, \tag{11}$$

and for the liquid phase:

$$\frac{\partial(\phi S)}{\partial t} - \operatorname{div}\left(\frac{k_{rw}}{\mu_w}\mathbf{K}\operatorname{grad} p_w\right) + \operatorname{div}(\phi S \mathbf{V}_s) = 0. \tag{12}$$

To close the system of equations (9)-(12) one usually considers a capillary pressure-saturation relation $p_c = p_c(S)$. In our case, when the paper-felt sandwich moves with about 2000 m/min between rolls, it is difficult to expect equilibrium conditions to be satisfied and considering dynamic capillary pressure is very reasonable. We have chosen the dynamic capillary pressure-saturation relationship derived by Hassanizadeh, Gray (1990, 1993a):

$$(p_a - p_w) - p_c^{stat} = -\tau \frac{D^s S}{Dt}, \tag{13}$$

where τ is a co-called material coefficient in $[Pa \cdot s]$, which still may depend on saturation and other parameters, p_c^{stat} is a prescribed static capillary pressure-saturation relation, $\frac{D^s S_w}{Dt}$ is the material derivative with respect to a reference frame fixed to the solid phase:

$$\frac{D^s S}{Dt} = \frac{\partial S}{\partial t} + \mathbf{V}_s \operatorname{grad} S. \tag{14}$$

Using (9)-(14) and the assumption $p_a \equiv 0$, we obtain the following system:

$$-\frac{\partial \phi}{\partial t} + \operatorname{div}((1-\phi)\mathbf{V}_s) = 0, \tag{15}$$

$$(1-\phi)\rho_s \left(\frac{\partial \mathbf{V}_s}{\partial t} + (\mathbf{V}_s \cdot \operatorname{grad})\mathbf{V}_s\right) - \operatorname{div}\mathbf{t}_s = \sum_{(\alpha)} \rho_\alpha^* \mathbf{F}_\alpha \tag{16}$$

$$\frac{\partial(\phi S)}{\partial t} - \operatorname{div}\left(\frac{k_{rw}}{\mu_w}\mathbf{K}\operatorname{grad} p_w\right) + \operatorname{div}(\phi S \mathbf{V}_s) = 0, \tag{17}$$

$$p_w + p_c^{stat} = \tau \frac{\partial S}{\partial t} + \tau \mathbf{V}_s \operatorname{grad} S. \tag{18}$$

In addition to the flow, one has to account also for the deformation of the porous media. This issue, in connection with flow model equipped with a standard (not dynamic) capillary pressure, is discussed in the PhD thesis of Rief (2005). Following the approach from Rief (2005), we treat consecutively the porous media deformation and the flow. For the deformation simulation we use the developments from Rief (2005) from where we find the distribution of the porosity, the thickness of the layer and the solid velocity. Thereby, from now on equations (15) and (16) can be skipped.

Back to the flow model, we are interested in the steady state solution, thus the partial derivatives with respect to time in (17) and (18) are set to zero and we obtain:

$$-\operatorname{div}\left(\frac{k_{rw}}{\mu_w}\mathbf{K}\operatorname{grad} p\right) + \operatorname{div}(\phi S \mathbf{V}_s) = 0, \tag{19}$$

$$p + p_c^{stat} = \tau \mathbf{V}_s \operatorname{grad} S, \tag{20}$$

where $p_w \equiv p$. Suitable boundary conditions have to be specified, see details below.

We should remark that the model (19), (20) suits only for unsaturated flow. Evaluation of the fully saturated regions is one of the issues of pressing section modeling. But in this work we are not concerned with this side of the problem. It is planned to include this effect in consideration in our future work.

2.2 Modeling one-dimensional flow

Here we should notice, that one-dimensional model can be considered only for one layer case. Therefore, it can not capture all effects, which present in two-dimensional model. The main effects, which are lost in one-dimensional case, are the movement of water between the layers in vertical direction and different press nip configurations. But one-dimensional model can be used to capture main behaviour of the pressure and saturation profiles and also to compare with existing laboratory experiments (Beck, 1983).

In this work we are concerned with the one-dimensional problem in machine direction with computational domain $\Omega = (A, B), B > A$ and boundary $\Gamma = \{x = A \cup x = B\}$ (see Figure 2). To obtain one-dimensional model we apply an averaging procedure in vertical direction (see Velten et al., 2000).

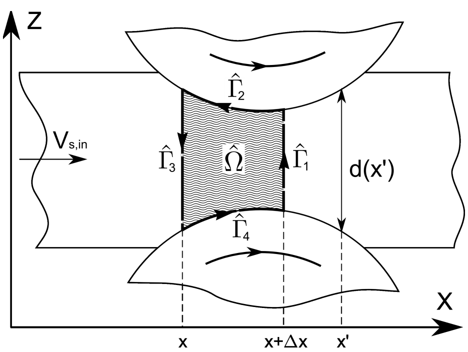

Fig. 3 Computational domain $\hat{\Omega}$ for obtaining a one-dimensional model

2.2.1 Averaging procedure for the mass conservation equation

Let us consider the integral form of the mass conservation equation for domain $\hat{\Omega} \subset \mathbb{R}^2$ (see Figure 3) in the case of no sources and no sinks and impermeable upper and lower boundaries:

$$\int_{\hat{\Omega}} \operatorname{div}(\phi S \mathbf{V}_w) d\sigma = 0,$$

where $\hat{\Omega} = \{(\hat{x}, \hat{z}) : \ \hat{x} \in [x, x + \Delta x], \ \hat{z} \in [f_l(\hat{x}), f_u(\hat{x})]\}$, $x \in [A, B]$, $\Delta x > 0$, $\Delta x \in \mathbb{R}_+$ is a fixed value, such that $x + \Delta x \in [A, B]$. Using Green's theorem one obtains the following integral over the boundary $\partial\hat{\Omega}$ with integration in the counterclockwise direction:

$$\oint_{\partial\hat{\Omega}} \phi S \mathbf{V}_w \cdot \mathbf{n} ds = 0, \tag{21}$$

where $\mathbf{n}$ is the outward unit normal of the boundary $\partial\hat{\Omega}$. The boundary $\partial\hat{\Omega}$ can be represented as (see Figure 3):

$$\partial\hat{\Omega} = \hat{\Gamma}_1 \cup \hat{\Gamma}_2 \cup \hat{\Gamma}_3 \cup \hat{\Gamma}_4,$$

where $\hat{\Gamma}_i \cap \hat{\Gamma}_j = \emptyset$ for all $i \neq j$. Let vector $\mathbf{V}_w$ have the following components $\mathbf{V}_w = (V_w^1, V_w^2)$. Then (21) yields:

$$\begin{aligned} 0 = \oint_{\partial\hat{\Omega}} \phi S \mathbf{V}_w \cdot \mathbf{n} ds &= \int_{\hat{\Gamma}_1} \phi S \mathbf{V}_w \cdot \mathbf{n}_1 ds + \int_{\hat{\Gamma}_2} \phi S \mathbf{V}_w \cdot \mathbf{n}_2 ds \\ &+ \int_{\hat{\Gamma}_3} \phi S \mathbf{V}_w \cdot \mathbf{n}_3 ds + \int_{\hat{\Gamma}_4} \phi S \mathbf{V}_w \cdot \mathbf{n}_4 ds \\ &= \int_{\mathcal{E}_{x+\Delta x}} \phi S V_w^1 ds - \int_{\mathcal{E}_x} \phi S V_w^1 ds, \end{aligned} \tag{22}$$

where $\mathcal{E}_x = \{(x,z) : z \in [f_l(x), f_u(x)]\}$ and the integrals over the boundaries $\hat{\Gamma}_2$ and $\hat{\Gamma}_4$ are equal to zero since in the two-dimensional case we imposed no-flow conditions for these boundaries ($\mathbf{V}_w \cdot \mathbf{n}|_{\hat{\Gamma}_2,\hat{\Gamma}_4} = 0$). We introduce a vertically averaged horizontal quantities $\hat{\phi}(x)$, $\hat{S}(x)$ and $\hat{V}_w^1(x)$ in the following way:

$$\begin{aligned} \hat{\phi}(x) &= \frac{1}{d(x)} \int_{\mathcal{E}_x} \phi(x,z) dz, \\ \hat{S}(x) &= \frac{1}{d(x)\hat{\phi}(x)} \int_{\mathcal{E}_x} \phi(x,z) S(x,z) dz, \\ \hat{V}_w^1(x) &= \frac{1}{d(x)\hat{\phi}(x)\hat{S}(x)} \int_{\mathcal{E}_x} \phi(x,z) S(x,z) V_w^1(x,z) dz, \end{aligned}$$

where $A \le x < x + \Delta x \le B$, $d(x) = f_u(x) - f_l(x) > 0$ is the thickness of the layer.

Remember that $\hat{\Gamma}_1 = \mathcal{E}_x$ and $\hat{\Gamma}_2 = \mathcal{E}_{x+\Delta x}$, equation (22) yields:

$$-\hat{\phi}(x)\hat{S}(x)\hat{V}_w^1(x)d(x) + \hat{\phi}(x+\Delta x)\hat{S}(x+\Delta x)\hat{V}_w^1(x+\Delta x)d(x+\Delta x) = 0. \tag{23}$$

Dividing (23) by Δx and passing to the limit $\Delta x \to 0$, one obtains:

$$\frac{\partial}{\partial x}\left(\hat{S}(x)\hat{\phi}(x)\hat{V}_w^1(x)d(x)\right) = 0. \tag{24}$$

Note, that x (see Figure 3) was chosen arbitrarily, therefore equation (24) is satisfied for any $x \in [A, B]$. Assuming that the intrinsic permeability tensor $\mathbf{K}$ has diagonal form:

$$\mathbf{K} = \begin{bmatrix} K(\phi) & 0 \\ 0 & \hat{K}(\phi) \end{bmatrix}$$

and taking into account Darcy's law (8) and omitting the hat over the averaged functions, the one-dimensional equation (19) reads:

$$-\frac{\partial}{\partial x}\left(d\frac{k_r(S)}{\mu}K(\phi)\frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial x}(d\phi S V_s) = 0, \quad x \in \Omega, \tag{25}$$

where V_s is considered as the x-component of averaged vector $\mathbf{V}_s$ and $\Omega = (A, B)$ is the one-dimensional computational domain.

In this work we consider the paper-felt sandwich, which is transported horizontally with constant speed $V_{s,in}$. Therefore, the x-component of the solid velocity, V_s, is does not depend on x and it is equal to $V_{s,in}$. From now on we consider V_s to be constant for our problem.

2.2.2 Averaging procedure for dynamic capillary pressure-saturation relation

Now we are concerned with the dynamic capillary pressure-saturation relation (20). For our problem we consider p_c^{stat} as a function of the saturation and the porosity: $p_c^{stat} = p_c^{stat}(S, \phi)$. Integration of the left hand side of (20) over $\hat{\Omega}$ yields:

$$\int_{\hat{\Omega}} p + p_c^{stat}(S,\phi) d\sigma \approx \left(\hat{p}_{\hat{\Omega}} + p_c^{stat}(\hat{S}_{\hat{\Omega}}, \hat{\phi}_{\hat{\Omega}})\right) m(\hat{\Omega}), \tag{26}$$

where $\hat{u}_{\hat{\Omega}}$ is the averaged over domain $\hat{\Omega}$ quantity defined by:

$$\hat{u}_{\hat{\Omega}} = \frac{1}{m(\hat{\Omega})} \int_{\hat{\Omega}} u d\sigma, \quad \lim_{\Delta x \to 0} \hat{u}_{\hat{\Omega}} = \hat{u}, \tag{27}$$

under assumption that $\hat{u}$ is a continuous function.

Let us integrate the right hand side of (20) over $\hat{\Omega}$:

$$\begin{aligned}
\int_{\hat{\Omega}} \tau \mathbf{V}_s \,\mathrm{grad}\, S d\sigma &= \int_{\hat{\Omega}} \mathrm{div}\,(\tau S \mathbf{V}_s)\, d\sigma - \int_{\hat{\Omega}} S\,\mathrm{div}\,(\tau \mathbf{V}_s)\, d\sigma \\
&\approx \oint_{\partial\hat{\Omega}} \tau S \mathbf{V}_s \cdot \mathbf{n} ds - \hat{S}_{\hat{\Omega}} \oint_{\partial\hat{\Omega}} \tau \mathbf{V}_s \cdot \mathbf{n} ds,
\end{aligned}$$

where $\hat{S}_{\hat{\Omega}}$ defined by (27). Remembering that V_s is the x-component of the vector $\mathbf{V}_s$ and that $\mathbf{V}_s \cdot \mathbf{n}|_{\hat{\Gamma}_2, \hat{\Gamma}_4} = 0$, we have:

$$\begin{aligned}
\int_{\hat{\Omega}} \tau \mathbf{V}_s \,\mathrm{grad}\, S d\sigma &\approx \int_{\hat{\Gamma}_1} \tau S \mathbf{V}_s \cdot \mathbf{n}_1 ds + \int_{\hat{\Gamma}_3} \tau S \mathbf{V}_s \cdot \mathbf{n}_3 ds \\
&\quad - \hat{S}_{\hat{\Omega}} \left(\int_{\hat{\Gamma}_1} \tau \mathbf{V}_s \cdot \mathbf{n}_1 ds + \int_{\hat{\Gamma}_3} \tau \mathbf{V}_s \cdot \mathbf{n}_3 ds \right) \\
&= \int_{\mathcal{E}_{x+\Delta x}} \tau S V_s ds - \int_{\mathcal{E}_x} \tau S V_s ds \\
&\quad - \hat{S}_{\hat{\Omega}} \left(\int_{\mathcal{E}_{x+\Delta x}} \tau V_s ds - \int_{\mathcal{E}_x} \tau V_s ds \right).
\end{aligned} \tag{28}$$

Defining functions $\hat{\tau}(x)$ and $\hat{S}(x)$ in the following way:

$$\begin{aligned}
\hat{\tau}(x) &= \frac{1}{d(x)} \int_{\mathcal{E}_x} \tau(x,z) dz, \\
\hat{S}(x) &= \frac{1}{d(x)\hat{\tau}(x)} \int_{\mathcal{E}_x} \tau(x,z) S(x,z) dz.
\end{aligned}$$

Then, equation (28) yields:

$$\begin{aligned}
\int_{\hat{\Omega}} \tau \mathbf{V}_s \,\mathrm{grad}\, S d\sigma &\approx \hat{\tau}(x+\Delta x) \hat{S}(x+\Delta x) V_s d(x+\Delta x) \\
&\quad - \hat{\tau}(x) \hat{S}(x) V_s d(x) \\
&\quad - \hat{S}_{\hat{\Omega}} \hat{\tau}(x+\Delta x) V_s d(x+\Delta x) \\
&\quad + \hat{S}_{\hat{\Omega}} \hat{\tau}(x) V_s d(x).
\end{aligned} \tag{29}$$

Dividing the right hand sides of equations (26) and (29) by Δx and passing to the limit $\Delta x \to 0$, one obtains:

$$d(x)\left(\hat{p}(x) + p_c^{stat}(\hat{S}(x), \hat{\phi}(x))\right) \\ = \frac{\partial}{\partial x}\left(\hat{\tau}(x)\hat{S}(x)V_s d(x)\right) - \hat{S}(x)\frac{\partial}{\partial x}\left(\hat{\tau}(x)V_s d(x)\right). \quad (30)$$

Transforming equation (30) we obtain:

$$p = \tau V_s \frac{\partial S}{\partial x} - p_c^{stat}, \quad x \in \Omega, \quad (31)$$

where the hats over the functions are omitted.

2.2.3 Boundary conditions

For the needs of the pressing section simulation, the boundary conditions have to be imposed. We prescribe Dirichlet boundary conditions for saturation at $x = A$:

$$S(A) = C_0, \quad (32)$$

We assume that these boundaries $x = A$ and $x = B$ of the computational domain Ω are far enough from the pressing roles and, thereby, there is no movement of water with respect to the solid structure. The stationary capillary pressure-saturation relation is satisfied and the following Dirichlet boundary condition is applied for pressure on the left boundary:

$$p(A) = -p_c^{stat}(C_0), \quad (33)$$

and since the equilibrium is reached with respect to the solid structure, on the right boundary we apply the Neumann boundary condition:

$$\left.\frac{\partial p}{\partial x}\right|_B = 0. \quad (34)$$

3 Discretization

Let N be the number of intervals into which our computational domain $\overline{\Omega} = [A, B]$ is divided. A vertex-centered grid is introduced for the pressure:

$$\mathcal{T}_p = \{x_i = ih, \ \ i = \overline{0, N}\},$$

where $h = (B - A)/N$ and $\overline{0, N} = 0, 1, ..., N$. The following grid is considered for the saturation:

$$\mathcal{T}_s = \{x_0 = A, \ x_{i+\frac{1}{2}} = \left(i + \frac{1}{2}\right)h, \ i = \overline{0, N-1}, \ x_N = B\}.$$

The grids for the pressure and the saturation are illustrated in Figure 4:

We discretize the system of equations (25), (31)-(34) by a finite volume method (see e.g. Eymard et al., 2006; Samarskij, 1971).

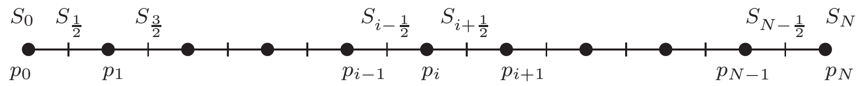

Fig. 4 Grid representation and numbering of variables

3.1 Discretization of the mass conservation equation

Let us integrate equation (25) over the interval $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$:

$$0 = -\int\limits_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial}{\partial x}\left(d\frac{k_r(S)}{\mu}K(\phi)\frac{\partial p}{\partial x}\right)dx + \int\limits_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial}{\partial x}(d\phi S V_s)dx =$$

$$w_{i+\frac{1}{2}} - w_{i-\frac{1}{2}} + V_s(d_{i+\frac{1}{2}}\phi_{i+\frac{1}{2}}S_{i+\frac{1}{2}} - d_{i-\frac{1}{2}}\phi_{i-\frac{1}{2}}S_{i-\frac{1}{2}}), \quad i = \overline{1, N-1},$$

where

$$w = -\frac{d \cdot k_r(S)K(\phi)}{\mu}\frac{\partial p}{\partial x}. \tag{35}$$

For all functions the notation $f_{i+\frac{1}{2}} = f(x_{i+\frac{1}{2}})$ is introduced. By integration of the transformed expression (35) over the interval $[x_{i-1}, x_i]$, we obtain:

$$\int\limits_{x_{i-1}}^{x_i} \frac{\partial p}{\partial x}dx = -\int\limits_{x_{i-1}}^{x_i} \frac{w\mu dx}{d \cdot k_r(S)K(\phi)}. \tag{36}$$

Assuming that $w(x) \approx \hat{w}_{i-\frac{1}{2}} = const$ for $x \in [x_{i-1}, x_i]$, equation (36) yields:

$$p_i - p_{i-1} \approx -\hat{w}_{i-\frac{1}{2}} \int\limits_{x_{i-1}}^{x_i} \frac{\mu dx}{d \cdot k_r(S)K(\phi)}.$$

From the last expression we find:

$$\hat{w}_{i-\frac{1}{2}} = -a_{i-\frac{1}{2}}\frac{p_i - p_{i-1}}{h}, \text{ where } a_{i-\frac{1}{2}} = \left(\frac{1}{h}\int\limits_{x_{i-1}}^{x_i} \frac{\mu dx}{d \cdot k_r(S)K(\phi)}\right)^{-1}.$$

Since the function $S(x)$ is unknown and the functions $\phi(x)$ and $d(x)$ can be represented only as discrete functions, we can not analytically find the coefficient $a_{i-\frac{1}{2}}$. Therefore, we use numerical integration, or more specifically, the midpoint rule:

$$a_{i-\frac{1}{2}} = \left(\frac{1}{h}\int\limits_{x_{i-1}}^{x_i} \frac{\mu dx}{d \cdot k_r(S)K(\phi)}\right)^{-1} \approx \left(\frac{1}{h}\frac{\mu h}{d_{i-\frac{1}{2}}k_r(S_{i-\frac{1}{2}})K(\phi_{i-\frac{1}{2}})}\right)^{-1},$$

$$\hat{a}_{i-\frac{1}{2}} = \frac{d_{i-\frac{1}{2}}k_r(S_{i-\frac{1}{2}})K(\phi_{i-\frac{1}{2}})}{\mu}. \tag{37}$$

Thus, the finite difference scheme for equation (25) is:

$$-\hat{a}_{i+\frac{1}{2}}\frac{p_{i+1} - p_i}{h} + \hat{a}_{i-\frac{1}{2}}\frac{p_i - p_{i-1}}{h} + V_s(d_{i+\frac{1}{2}}\phi_{i+\frac{1}{2}}S_{i+\frac{1}{2}} - d_{i-\frac{1}{2}}\phi_{i-\frac{1}{2}}S_{i-\frac{1}{2}}) = 0,$$
$$i = \overline{1, N-1}. \tag{38}$$

3.2 Discretization of the equation for capillary pressure

In the numerical experiments below we consider the material parameter τ from (31) to be constant. But we perform the discretization procedure keeping the assumption $\tau = \tau(x)$, in order not to lose generality.

Now we are concerned with equation (31). We integrate equation (31) over the interval $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ for $i = \overline{1, N-1}$:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} p dx = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \tau V_s \frac{\partial S}{\partial x} dx - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} p_c^{stat} dx, \tag{39}$$

We consider the left-hand side of (39):

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} p dx \approx h p_i,$$

The first term on the right-hand side of (39) yields:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \tau V_s \frac{\partial S}{\partial x} dx \approx V_s \tau_{i+\frac{1}{2}} \left(S_{i+\frac{1}{2}} - S_{i-\frac{1}{2}} \right).$$

The second term on the right-hand side of (39) yields:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} p_c^{stat}(S, \phi) dx = h p_c^{stat}(S_{i+\frac{1}{2}}, \phi_{i+\frac{1}{2}}).$$

Summarizing, the numerical scheme for (31) takes the form:

$$p_i = \frac{V_s}{h} \tau_{i+\frac{1}{2}} \left(S_{i+\frac{1}{2}} - S_{i-\frac{1}{2}} \right) - p_c^{stat}(S_{i+\frac{1}{2}}, \phi_{i+\frac{1}{2}}), \quad i = \overline{1, N-1}. \tag{40}$$

3.3 Discretization of the boundary conditions

Integrating equation (25) over the interval $[x_{N-\frac{1}{2}}, x_N]$ we obtain

$$\begin{aligned} &\int_{x_{N-\frac{1}{2}}}^{x_N} -\frac{\partial}{\partial x} \left(d \frac{k_r(S) K(\phi)}{\mu} \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial x} (d \phi S V_s) dx \\ &\qquad = - \left(d \frac{k(S) K(\phi)}{\mu} \frac{\partial p}{\partial x} \right) \Bigg|_{x_{N-\frac{1}{2}}}^{x_N} + \left(d \phi S V_s \right)\Big|_{x_{N-\frac{1}{2}}}^{x_N}. \end{aligned}$$

Using the boundary condition (34) and central differences for the discretization of the partial derivatives of the pressure we obtain the following approximation:

$$d_{N-\frac{1}{2}}\frac{k_r(S_{N-\frac{1}{2}})K(\phi_{N-\frac{1}{2}})}{\mu}\frac{p_N-p_{N-1}}{h}+V_s(d_N\phi_N S_N-d_{N-\frac{1}{2}}\phi_{N-\frac{1}{2}}S_{N-\frac{1}{2}})=0$$

or

$$\hat{a}_{N-\frac{1}{2}}\frac{p_N-p_{N-1}}{h}+V_s(d_N\phi_N S_N-d_{N-\frac{1}{2}}\phi_{N-\frac{1}{2}}S_{N-\frac{1}{2}})=0,$$

where $\hat{a}_{N-\frac{1}{2}}$ is defined by equation (37). This is a second-order approximation for the Neumann boundary condition (34) for the pressure. The Dirichlet boundary conditions (32) and (33) are discretized exactly:

$$p_0=-p_c^{stat}(C_0),\quad S_0=C_0.$$

Two more equations are needed to close the system of discretized equations. The first one is obtained by integrating equation (31) over the interval $[x_0, x_{\frac{1}{2}}]$:

$$\int_{x_0}^{x_{\frac{1}{2}}} p dx=\int_{x_0}^{x_{\frac{1}{2}}} V_s\tau\frac{\partial S}{\partial x}dx-\int_{x_0}^{x_{\frac{1}{2}}} p_c^{stat}dx.$$

$$\int_{x_0}^{x_{\frac{1}{2}}} p dx\approx\frac{h}{2}p_0,$$

$$\int_{x_0}^{x_{\frac{1}{2}}} V_s\tau\frac{\partial S}{\partial x}dx\approx V_s\tau_{\frac{1}{2}}\left(S_{\frac{1}{2}}-S_0\right),$$

$$\int_{x_0}^{x_{\frac{1}{2}}} p_c^{stat}(S,\phi)dx\approx\frac{h}{2}p_c^{stat}(S_{\frac{1}{2}},\phi_{\frac{1}{2}}).$$

Finally, we obtain:

$$p_0=\frac{2V_s}{h}\tau_{\frac{1}{2}}\left(S_{\frac{1}{2}}-S_0\right)-p_c^{stat}(S_{\frac{1}{2}},\phi_{\frac{1}{2}}). \tag{41}$$

Integrating (31) over the interval $[x_{N-\frac{1}{2}}, x_N]$, it yields:

$$p_N=\frac{2V_s}{h}\tau_N(S_N-S_{N-\frac{1}{2}})-p_c^{stat}(S_N,\phi_N). \tag{42}$$

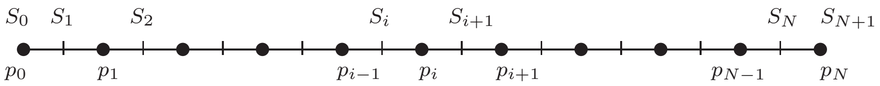

Fig. 5 Renumbering of variables

3.4 Finite difference scheme

To write the finite difference scheme we change the numbering of saturation values in the following way: $S_0 \to S_0$, $S_{\frac{1}{2}} \to S_1$, ..., $S_{i-\frac{1}{2}} \to S_i$, $S_{i+\frac{1}{2}} \to S_{i+1}$, ..., $S_{N-\frac{1}{2}} \to S_N$, $S_N \to S_{N+1}$ (see Figure 5).

Finally, we can write down the following system of $(2N+3)$ equations with respect to $(2N+3)$ unknowns:

$$p_0 = -p_c^{stat}(C_0), \tag{43}$$

$$-\hat{a}_{i+1}\frac{p_{i+1}-p_i}{h} + \hat{a}_i\frac{p_i - p_{i-1}}{h} + V_s(d_{i+1}\phi_{i+1}S_{i+1} - d_i\phi_i S_i) = 0,\ i = \overline{1, N-1}, \tag{44}$$

$$\hat{a}_N\frac{p_N - p_{N-1}}{h} + V_s(d_{N+1}\phi_{N+1}S_{N+1} - d_N\phi_N S_N) = 0, \tag{45}$$

$$\hat{a}_i = d_i\frac{k_r(S_i)K(\phi_i)}{\mu},\ i = \overline{1, N}, \tag{46}$$

$$S_0 = C_0, \tag{47}$$

$$p_0 = \frac{2V_s}{h}\tau_1\left(S_1 - S_0\right) - p_c^{stat}(S_1, \phi_1). \tag{48}$$

$$p_i = \frac{V_s}{h}\tau_{i+1}\left(S_{i+1} - S_i\right) - p_c^{stat}(S_{i+1}, \phi_{i+1}),\quad i = \overline{1, N-1}, \tag{49}$$

$$p_N = \frac{2V_s}{h}\tau_{N+1}(S_{N+1} - S_N) - p_c^{stat}(S_{N+1}, \phi_{N+1}). \tag{50}$$

In the following we will also consider the case when the material coefficient τ equals to zero. Therefore, we present here the finite difference scheme for this case.

When the coefficient τ in (31) is equal to zero the initial system of equations (25), (31) becomes a nonlinear equation (25) with boundary conditions (33), (34), where the pressure $\mathbf{p} = (p_0, p_1, \ldots, p_N)$ is considered as unknown variable. In this case saturation is a dependent variable and expressed as an analytical function of the pressure.

Setting the coefficient τ to zero in discretized system (43)-(50) we have equations (43)-(46) together with:

$$S_0 = C_0, \tag{51}$$

$$p_i = -p_c^{stat}(S_{i+1}, \phi_{i+1}),\quad i = \overline{0, N}. \tag{52}$$

Let us assume that function $p_c^{stat}(S, \phi)$ is a continuous function such that $p_c^{stat} : (S_*, 1] \times (0, 1) \leftrightarrow \mathbb{R}^+$ and it is a bijection, where $S_* \in \mathbb{R}$ and $S_* > 0$. Then, it has an inverse with respect to S function $\left(p_c^{stat}\right)^{-1}(p, \phi)$. Therefore, equations (52) can be written down in the following form:

$$S_{i+1} = \left(p_c^{stat}\right)^{-1}\left(-p_i, \phi_{i+1}\right),\quad i = \overline{0, N}. \tag{53}$$

Remark 1 In case of standard capillary pressure-saturation relation the saturation can also be approximated in the following way:

$$S_0 = C_0, \tag{54}$$

$$S_{i+1} = \left(p_c^{stat}\right)^{-1}\left(-\frac{1}{2}\left(p_i + p_{i+1}\right), \phi_{i+1}\right), \quad i = \overline{0, N-1}, \tag{55}$$

$$S_{N+1} = \left(p_c^{stat}\right)^{-1}\left(-p_N, \phi_{N+1}\right). \tag{56}$$

This approximation gives us finite difference scheme with second order accuracy. But the numerical simulations result in nonphysical oscillations (see Appendix 6). It happens because of the approximation of the convective term in (25) by central differences.

In the following we choose to have first order accuracy and solution without oscillations.

4 Solution of the nonlinear system by Newton's method

The discretization (43)-(50) is a system of nonlinear algebraic equations. In this section we will recall Newton's method and will discuss how we apply it when solving the reduced system (with standard capillary pressure) and when we solve the full nonlinear system (43)-(50).

4.1 Introduction to Newton's method for a nonlinear system

A system of nonlinear equations is expressed in the form $\mathbf{F}(\mathbf{x}) = 0$, where $\mathbf{F}$ is a vector-valued function of the vector variable $\mathbf{x}$ such that $\mathbf{F} : R^n \to R^n$. Given an estimate $\mathbf{x}^{(k)}$ of a solution $\mathbf{x}^*$, Newton's method computes the next iterate $\mathbf{x}^{(k+1)}$ by setting the local linear approximation to $\mathbf{F}$ at $\mathbf{x}^{(k+1)}$ to zero, and solving for the correction $\Delta\mathbf{x}^{(k+1)} = \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}$:

$$\mathbf{F}(\mathbf{x}^{(k+1)}) = \mathbf{F}(\mathbf{x}^{(k)}) + \mathbf{J}(\mathbf{x}^{(k)})(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = 0,$$

$$\mathbf{J}(\mathbf{x}^{(k)})\Delta\mathbf{x}^{(k+1)} = -\mathbf{F}(\mathbf{x}^{(k)}),$$

$$\Delta\mathbf{x}^{(k+1)} = -\mathbf{J}^{-1}(\mathbf{x}^{(k)})\mathbf{F}(\mathbf{x}^{(k)}),$$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \Delta\mathbf{x}^{(k+1)}.$$

In this calculation, $\mathbf{J}(\mathbf{x}^{(k)})$ is the Jacobian matrix of $\mathbf{F}$ at $\mathbf{x}^{(k)}$. Here, we assume that $\mathbf{J}$ is nonsingular matrix, otherwise, the Newton step is undefined. For more details of Newton's method (see Deuflhard, 2004; Kelley, 1995).

4.2 Problem with stationary capillary pressure-saturation relation

At first we consider simpler problem with the standard stationary capillary pressure-saturation relation. In this subsection we derive the analytical form of the function $\mathbf{F} = (F_0, F_1, \dots F_N)^T$ and the Jacobian $\mathbf{J}_F$, which are necessary to solve the problem.

To apply Newton's method, we transform (43)-(46) as follows:

$$F_0 = p_0 + p_c^{stat}(C_0), \tag{57}$$

$$\begin{aligned} F_i = & -d_{i+1}\frac{K(\phi_{i+1})k_r(S_{i+1})}{\mu}\frac{p_{i+1}-p_i}{h} + d_i\frac{K(\phi_i)k_r(S_i)}{\mu}\frac{p_i-p_{i-1}}{h} \\ & + V_s(d_{i+1}\phi_{i+1}S_{i+1} - d_i\phi_i S_i), \quad i = \overline{1, N-1}, \end{aligned} \tag{58}$$

$$F_N = d_N\frac{K(\phi_N)k_r(S_N)}{\mu}\frac{p_N - p_{N-1}}{h} + V_s(d_{N+1}\phi_{N+1}S_{N+1} - d_N\phi_N S_N), \tag{59}$$

where S_i, $i = \overline{1, N+1}$ are defined by (51), (53).

Hence, the Jacobian reads:

$$\mathbf{J}_F = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ \frac{\partial F_1}{\partial p_0} & \frac{\partial F_1}{\partial p_1} & \frac{\partial F_1}{\partial p_2} & 0 & \dots & 0 & 0 \\ 0 & \frac{\partial F_2}{\partial p_1} & \frac{\partial F_2}{\partial p_2} & \frac{\partial F_2}{\partial p_3} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & \frac{\partial F_N}{\partial p_{N-1}} & \frac{\partial F_N}{\partial p_N} \end{pmatrix}, \tag{60}$$

with the following entries:

$$\begin{aligned} \frac{\partial F_i}{\partial p_{i-1}} = & \, d_i\frac{K(\phi_i)}{\mu h}\left((k_r(S_i))'_{p_{i-1}}(p_i - p_{i-1}) - k_r(S_i)\right) \\ & - V_s d_i \phi_i (S_i)'_{p_{i-1}}, \quad i = \overline{1, N-1}, \end{aligned} \tag{61}$$

$$\begin{aligned} \frac{\partial F_i}{\partial p_i} = & -d_{i+1}\frac{K(\phi_{i+1})}{\mu h}\left((k_r(S_{i+1}))'_{p_i}(p_{i+1} - p_i) - k_r(S_{i+1})\right) \\ & + d_i\frac{K(\phi_i)k_r(S_i)}{\mu h} + V_s d_{i+1}\phi_{i+1}(S_{i+1})'_{p_i}, \quad i = \overline{1, N-1}, \end{aligned} \tag{62}$$

$$\frac{\partial F_i}{\partial p_{i+1}} = -d_{i+1}\frac{K(\phi_{i+1})k_r(S_{i+1})}{\mu h}, \quad i = \overline{1, N-1}, \tag{63}$$

$$\begin{aligned} \frac{\partial F_N}{\partial p_{N-1}} = & \, d_N\frac{K(\phi_N)}{\mu h}\left((k_r(S_N))'_{p_{N-1}}(p_N - p_{N-1}) - k_r(S_N)\right) \\ & - V_s d_N \phi_N (S_N)'_{p_{N-1}}, \end{aligned} \tag{64}$$

$$\frac{\partial F_N}{\partial p_N} = d_N\frac{K(\phi_N)k_r(S_N)}{\mu h} + V_s d_{N+1}\phi_{N+1}(S_{N+1})'_{p_N}. \tag{65}$$

Let k be the iteration index. Then, after the k-th iteration we obtain the following linear system:

$$\mathbf{J}_F^{(k)}\Delta\mathbf{p}^{(k+1)} = -\mathbf{F}^{(k)}, \tag{66}$$

where

$$\begin{aligned}\mathbf{F}^{(k)} &= \mathbf{F}(\mathbf{p}^{(k)}),\\ \mathbf{J}_F^{(k)} &= \mathbf{J}_F(\mathbf{p}^{(k)}),\\ \varDelta\mathbf{p}^{(k+1)} &= \mathbf{p}^{(k+1)} - \mathbf{p}^{(k)}\end{aligned}$$

and $\mathbf{p}^{(k)} = (p_0^{(k)}, p_1^{(k)}, \ldots, p_N^{(k)})$ is an approximation of the solution at the k-th iteration. The threediagonal system (66) is solved using the Thomas algorithm (Samarskij, 1971).

As the numerical experiments show the above described algorithms give convergent methods. But the theoretical studies for Newton's method for our problem still has to be done. There are works which prove the convergence of Newton's method for a finite volume scheme of nonlinear elliptic problems (e.g. Chatzipantelidis et al., 2005; Douglas, Dupont, 1979). This problem is similar to ours. The diffusive term is the same, but the convective term still has to be included in the theoretical studies.

4.3 Problem with dynamic capillary pressure-saturation relation

Let us consider now the full system of nonlinear algebraic equations (43)-(50), corresponding to the case of dynamic capillary pressure, $\tau \neq 0$. For convenience, let us write this system in the following form:

$$\begin{aligned}\mathbf{F}(\mathbf{p}, \mathbf{S}) &= 0,\\ \mathbf{G}(\mathbf{p}, \mathbf{S}) &= 0.\end{aligned}$$

This is the system of two equations with two vector unknowns, the pressure $\mathbf{p}$ and the saturation $\mathbf{S}$. The direct application of Newton's method to this system reads:

$$\begin{pmatrix} \left(\frac{\partial \mathbf{F}}{\partial \mathbf{p}}\right)^{(k)} & \left(\frac{\partial \mathbf{F}}{\partial \mathbf{S}}\right)^{(k)} \\ \left(\frac{\partial \mathbf{G}}{\partial \mathbf{p}}\right)^{(k)} & \left(\frac{\partial \mathbf{G}}{\partial \mathbf{S}}\right)^{(k)} \end{pmatrix} \begin{pmatrix} \varDelta\mathbf{p}^{(k+1)} \\ \varDelta\mathbf{S}^{(k+1)} \end{pmatrix} = - \begin{pmatrix} \mathbf{F}^{(k)} \\ \mathbf{G}^{(k)} \end{pmatrix}, \tag{67}$$

$$\begin{pmatrix} \mathbf{p}^{(k+1)} \\ \mathbf{S}^{(k+1)} \end{pmatrix} = \begin{pmatrix} \mathbf{p}^{(k)} \\ \mathbf{S}^{(k)} \end{pmatrix} + \begin{pmatrix} \varDelta\mathbf{p}^{(k+1)} \\ \varDelta\mathbf{S}^{(k+1)} \end{pmatrix}. \tag{68}$$

In case of the stationary capillary pressure-saturation relation at each Newton iteration we had a linear system with $(N+1)$ unknowns. The iteration process (67), (68) produces a linear system with $(2N+3)$ unknowns. Increased size of the system slows down the computational process as compared with the first case and uses a lot of machine memory. Therefore, we want to develop an algorithm, which will solve one equation at a time.

To achieve the convergence of the iterative process solving one equation at a time we perform the following procedure. For the first system of equations, the discretized mass conservation equation, we develop a new system of equations $\mathbf{F}^*$ and solve it w.r.t. the pressure $\mathbf{p}$ (see Section 4.3.1). The second system of equations $\mathbf{G}^*$, the discretized dynamic capillary pressure-saturation relation, is used to find distribution of the saturation $\mathbf{S}$ (see Section 4.3.2). So one step of the iteration process is presented in the following matrix way:

$$\begin{pmatrix} \frac{\partial \mathbf{F}^*}{\partial \mathbf{p}}(\mathbf{p}^{(k)},\mathbf{S}^{(k)}) & 0 \\ 0 & \frac{\partial \mathbf{G}^*}{\partial \mathbf{S}}(\mathbf{p}^{(k+1)},\mathbf{S}^{(k)}) \end{pmatrix} \begin{pmatrix} \Delta\mathbf{p}^{(k+1)} \\ \Delta\mathbf{S}^{(k+1)} \end{pmatrix} = - \begin{pmatrix} \mathbf{F}^*(\mathbf{p}^{(k)},\mathbf{S}^{(k)}) \\ \mathbf{G}^*(\mathbf{p}^{(k+1)},\mathbf{S}^{(k)}) \end{pmatrix}.$$

In the following we will omit the index "$*$" and will consider $\mathbf{F}$ for the modified mass conservation equation and $\mathbf{G}$ for the dynamic capillary pressure-saturation relation. Then, assuming that the initial guesses $\mathbf{p}^{(0)}$ and $\mathbf{S}^{(0)}$, the algorithm for the iteration process yields:

– Solve the linear system of equations:

$$\frac{\partial \mathbf{F}}{\partial \mathbf{p}}\left(\mathbf{p}^{(k)},\mathbf{S}^{(k)}\right)\Delta\mathbf{p}^{(k+1)} = -\mathbf{F}\left(\mathbf{p}^{(k)},\mathbf{S}^{(k)}\right).$$

– Update the pressure:

$$\mathbf{p}^{(k+1)} = \mathbf{p}^{(k)} + \Delta\mathbf{p}^{(k+1)}.$$

– Solve the linear system of equations:

$$\frac{\partial \mathbf{G}}{\partial \mathbf{S}}\left(\mathbf{p}^{(k+1)},\mathbf{S}^{(k)}\right)\Delta\mathbf{S}^{(k+1)} = -\mathbf{G}\left(\mathbf{p}^{(k+1)},\mathbf{S}^{(k)}\right).$$

– Update the saturation:

$$\mathbf{S}^{(k+1)} = \mathbf{S}^{(k)} + \Delta\mathbf{S}^{(k+1)}.$$

The numerical experiment shows that this algorithm gives us a convergent iterative process. Its theoretical investigations is a subject of further research.

4.3.1 The mass conservation equation

To develop a new system of equations $\mathbf{F}$ we carry out the following equivalent transformation procedure. We express $p_c^{stat}(S_i,\phi_i),\ i=\overline{1,N+1}$ from equations (48)-(50):

$$\begin{aligned} p_c^{stat}(S_1,\phi_1) &= \frac{2V_s}{h}\tau_1(S_1-S_0)-p_0, \\ p_c^{stat}(S_{i+1},\phi_{i+1}) &= \frac{V_s}{h}\tau_{i+1}\left(S_{i+1}-S_i\right)-p_i, \quad i=\overline{1,N-1}, \\ p_c^{stat}(S_{N+1},\phi_{N+1}) &= \frac{2V_s}{h}\tau_{N+1}(S_{N+1}-S_N)-p_N. \end{aligned}$$

The right-hand sides of these equations will be defined as functions:

$$g_i = g_i(S_i,S_{i-1},p_{i-1}), \quad i=\overline{1,N+1}.$$

Hence, we have:

$$p_c^{stat}(S_i,\phi_i) = g_i(S_i,S_{i-1},p_{i-1}), \quad i=\overline{1,N+1}. \tag{69}$$

In section 3.4 we have already made some assumption on the function $p_c^{stat} = p_c^{stat}(S,\phi)$. Using these assumptions, we obtain from (69) the following:

$$S_i = \left(p_c^{stat}\right)^{-1}\left(g_i(S_i,S_{i-1},p_{i-1}),\phi_i\right), \quad i=\overline{1,N+1}.$$

This system of equation is equivalent to the system (48)-(50). Let us assume that after some k-th iteration we have approximations $\mathbf{p}^{(k)}$ and $\mathbf{S}^{(k)}$. Then an intermediate iterate $\hat{\mathbf{S}}^{(k)}$ is defined by:

$$\hat{S}_i^{(k)} = \left(p_c^{stat}\right)^{-1} (g_i(S_i^{(k)}, S_{i-1}^{(k)}, p_{i-1}^{(k)}), \phi_i), \;\; i = \overline{1, N+1}. \tag{70}$$

Omitting the iteration indexes (k), we introduce $\hat{S}_i$, $i = \overline{0, N+1}$, where $\hat{S}_0 = C_0$, defined by (70) in the discretized mass conservation equations (see (43)-(46)) and represent them in a form suitable for Newton's method, we obtain equations the same as (57)-(59) with the only difference that instead of S we have $\hat{S}$. This remark is also true for the Jacobian entries (61)-(65). But for consistency we write down these equations once again:

$$\begin{aligned}
F_0 &= p_0 + p_c^{stat}(C_0),\\
F_i &= -d_{i+1}\frac{K(\phi_{i+1})k_r(\hat{S}_{i+1})}{\mu}\frac{p_{i+1}-p_i}{h} + d_i\frac{K(\phi_i)k_r(\hat{S}_i)}{\mu}\frac{p_i-p_{i-1}}{h}\\
&\quad + V_s(d_{i+1}\phi_{i+1}\hat{S}_{i+1} - d_i\phi_i\hat{S}_i), \;\; i = \overline{1, N-1},\\
F_N &= d_N\frac{K(\phi_N)k_r(\hat{S}_N)}{\mu}\frac{p_N - p_{N-1}}{h} + V_s(d_{N+1}\phi_{N+1}\hat{S}_{N+1} - d_N\phi_N\hat{S}_N).
\end{aligned}$$

Then, the Jacobian $\mathbf{J}_F$ defined by (60) has the following entries:

$$\begin{aligned}
\frac{\partial F_i}{\partial p_{i-1}} &= d_i\frac{K(\phi_i)}{\mu h}\left((k_r(\hat{S}_i))'_{p_{i-1}}(p_i - p_{i-1}) - k_r(\hat{S}_i)\right)\\
&\quad - V_s d_i\phi_i(\hat{S}_i)'_{p_{i-1}}, \;\; i = \overline{1, N-1},\\
\frac{\partial F_i}{\partial p_i} &= -d_{i+1}\frac{K(\phi_{i+1})}{\mu h}\left((k_r(\hat{S}_{i+1}))'_{p_i}(p_{i+1} - p_i) - k_r(S_{i+1})\right)\\
&\quad + d_i\frac{K(\phi_i)k_r(\hat{S}_i)}{\mu h} + V_s d_{i+1}\phi_{i+1}(\hat{S}_{i+1})'_{p_i}, \;\; i = \overline{1, N-1},\\
\frac{\partial F_i}{\partial p_{i+1}} &= -d_{i+1}\frac{K(\phi_{i+1})k_r(\hat{S}_{i+1})}{\mu h}, \;\; i = \overline{1, N-1},\\
\frac{\partial F_N}{\partial p_{N-1}} &= d_N\frac{K(\phi_N)}{\mu h}\left((k_r(\hat{S}_N))'_{p_{N-1}}(p_N - p_{N-1}) - k_r(\hat{S}_N)\right)\\
&\quad - V_s d_N\phi_N(\hat{S}_N)'_{p_{N-1}},\\
\frac{\partial F_N}{\partial p_N} &= d_N\frac{K(\phi_N)k_r(\hat{S}_N)}{\mu h} + V_s d_{N+1}\phi_{N+1}(\hat{S}_{N+1})'_{p_N}.
\end{aligned}$$

where

$$\begin{aligned}
(k_r(\hat{S}_i))'_{p_{i-1}} &= (k_r(\hat{S}_i))'_{\hat{S}_i}(\hat{S}_i)'_{g_i}(g_i)'_{p_{i-1}}, \;\; i = \overline{1, N+1},\\
(\hat{S}_i)'_{p_{i-1}} &= (\hat{S}_i)'_{g_i}(g_i)'_{p_{i-1}}, \;\; i = \overline{1, N+1}.
\end{aligned}$$

4.3.2 Equation for the capillary pressure

The discretized equations for capillary pressure (47)-(50) in a form suitable for Newton's method read:

$$\begin{aligned}
G_0 &= S_0 - C_0,\\
G_1 &= -p_0 - p_c^{stat}(S_1,\phi_1) + \frac{2V_s}{h}\tau_1(S_1 - S_0),\\
G_i &= -p_{i-1} - p_c^{stat}(S_i,\phi_i) + \frac{V_s}{h}\tau_i\left(S_i - S_{i-1}\right),\quad i=\overline{2,N},\\
G_{N+1} &= -p_N - p_c^{stat}(S_{N+1},\phi_{N+1}) + \frac{2V_s}{h}\tau_{N+1}(S_{N+1} - S_N).
\end{aligned}$$

Then the Jacobian for Newton's method takes the form:

$$\mathbf{J}_G = \begin{pmatrix}
1 & 0 & 0 & \dots & 0 & 0\\
\frac{\partial G_1}{\partial S_0} & \frac{\partial G_1}{\partial S_1} & 0 & \dots & 0 & 0\\
0 & \frac{\partial G_2}{\partial S_1} & \frac{\partial G_2}{\partial S_2} & \dots & 0 & 0\\
\dots & \dots & \dots & \dots & \dots & \dots\\
0 & 0 & 0 & \dots & \frac{\partial G_{N+1}}{\partial S_N} & \frac{\partial G_{N+1}}{\partial S_{N+1}}
\end{pmatrix},$$

where:

$$\begin{aligned}
\frac{\partial G_i}{\partial S_{i-1}} &= -\frac{V_s}{h}\tau_i\ \ i=\overline{2,N},\\
\frac{\partial G_i}{\partial S_i} &= -\left(p_c^{stat}(S_i,\phi_i)\right)'_{S_i} + \frac{V_s}{h}\tau_i,\quad i=\overline{2,N},\\
\frac{\partial G_i}{\partial S_{i-1}} &= -\frac{2V_s}{h}\tau_i,\quad i=\{1,N+1\};\\
\frac{\partial G_i}{\partial S_i} &= -\left(p_c^{stat}(S_i,\phi_i)\right)'_{S_i} + \frac{2V_s}{h}\tau_i,\quad i=\{1,N+1\}.
\end{aligned}$$

At the k-th iteration obtained the following linear system:

$$\mathbf{J}_G^{(k)}\Delta\mathbf{S}^{(k+1)} = -\mathbf{G}^{(k)}$$

and can be solved directly:

$$\begin{cases}
\Delta S_0^{(k+1)} = 0,\\
\Delta S_1^{(k+1)} = -G_1^{(k)}\cdot\left(\left(\dfrac{\partial G_1}{\partial S_1}\right)^{(k)}\right)^{-1},\\
\Delta S_{i+1}^{(k+1)} = \left(-G_{i+1}^{(k)} - \left(\dfrac{\partial G_{i+1}}{\partial S_i}\right)^{(k)}\cdot\Delta S_i^{(k+1)}\right)\left(\left(\dfrac{\partial G_{i+1}}{\partial S_{i+1}}\right)^{(k)}\right)^{-1},\quad i=\overline{1,N}.
\end{cases}$$

Table 1 Experimental Data (Rief, 2007)

Variable	Definition	Dimension	Value
k_r	relative permeability	$-$	S^b
b	parameter for relative permeability	$-$	3.5
K	intrinsic permeability	$[m^2]$	$K_0 \frac{\phi^3}{(1-\phi)^2}$
K_0	parameter for intrinsic permeability	$[m^2]$	$5e-12$
μ	viscosity	$[Pa \cdot s]$	0.0008
V_s	solid velocity	$[m/s]$	1.667
p_c^{stat}	static capillary pressure	$[Pa]$	$a(\phi-1)\left(\frac{1}{S-S_r}-\frac{1}{1-S_r}\right)^{1/2}$
a	parameter for capillary pressure	$[Pa]$	$\frac{P_0}{1-\phi_0}\left(\frac{1}{C_0-S_r}-\frac{1}{1-S_r}\right)^{-1/2}$
S_r	residual saturation	$-$	0.1
P_0	initial pressure	$[Pa]$	-5000
C_0	initial saturation	$-$	0.5
ϕ_0	initial porosity	$-$	0.875
A	the left boundary of the computational domain Ω	$[m]$	-0.05
B	the right boundary of the computational domain Ω	$[m]$	0.05

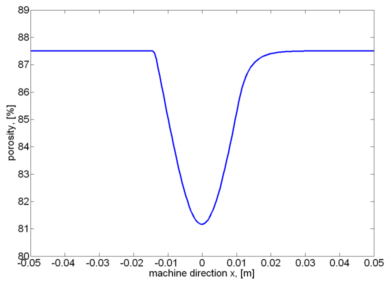

Fig. 6 Distribution of porosity

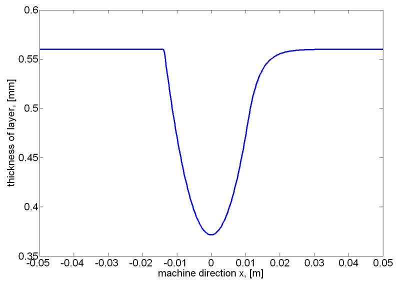

Fig. 7 Thickness of layer

5 Numerical experiments

The goal of this section is to study the influence of the dynamic capillary pressure on the behavior of the solution for different values of τ and to find out how accurate the obtained one-dimensional model is. Numerical experiments were carried out for parameters which are typical for a paper layer during a production process. The distribution of porosity and thickness of the layer are obtained from the model realized in Rief (2005) (see Figures 6 and 7). The remaining data, needed for computational experiments, is presented in Table 1.

5.1 Numerical experiment for the different values of the coefficient τ

Simulation results for the material coefficients between $\tau = 0$ and 10^4 $Pa \cdot s$ are presented. This range of the parameter τ was chosen, because for $\tau = 0$ $Pa \cdot s$ we have the standard model with $p = -p_c^{stat}$, then we increase this value by a factor 10 for each new experiment until we observe the significant difference for both output

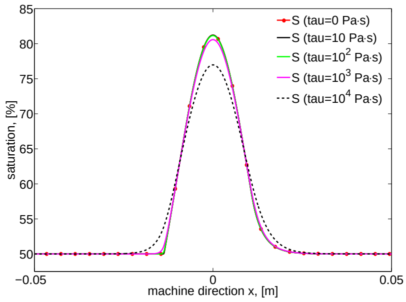

Fig. 8 Distributions of saturation for different values of τ

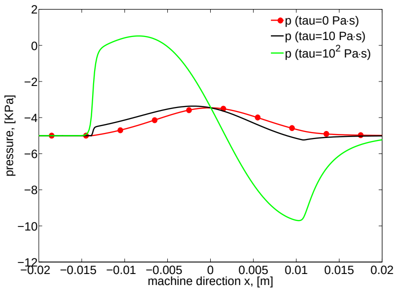

Fig. 9 Distributions of pressure for τ equal $0, 10, 100\ Pa \cdot s$

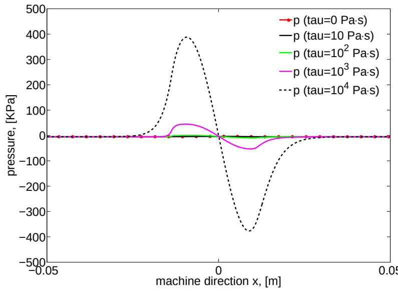

Fig. 10 Distributions of pressure for different values of τ

functions, pressure and saturation. We want to notice that this range of τ does not contradict the real values of the material coefficient which were observed in different experiments (Hassanizadeh et al., 2002; Manthey, 2006).

The distribution of porosity and the thickness of the layer, which are used as input data, are presented in Figures 6 and 7. Results are shown in Figure 8, where saturation S is plotted as a function of x-coordinate. Five different curves are represented, they correspond to values of τ equal to 0, 10, 10^2, 10^3 and $10^4\ Pa \cdot s$. The case when τ is equal to zero represents the static capillary pressure curve. Figure 8 shows that for this set of input parameters, there is no significant difference in saturation for all values except $\tau = 10^4\ Pa \cdot s$. But for pressure (see Figure 9 and 10) we observe that the changes start already from $\tau = 10\ Pa \cdot s$. Thus, we conclude that the dynamic capillary pressure model included in the simulation of the pressing problems influences the solution.

It was experimentally verified by Beck (1983) that the pressure peak locates before the center of the pressing zone. The model with the standard capillary pressure-saturation relation ($\tau = 0\ Pa \cdot s$) gives absolutely symmetric distribution of the pressure with respect to nip centers. But when we include the dynamic effect in the capillary pressure a shift of the peak is observed. Moreover, the behaviour of the pressure profile obtained by our model corresponds to the experimental data announced in Beck (1983). It means that we observe the same decreasing of the pressure below the initial value behind the center of the pressing zone and before the equilibrium w.r.t. the moving solid phase is reached (see Figure 9 and Beck (1983)).

According to the behaviour of pressure from the experimental data (see Beck, 1983) we expect that the material coefficient τ has an order $10 - 10^2$ $Pa \cdot s$ for the felt which is used in our numerical experiment. Nevertheless, results are presented for the range of τ from 0 to 10^4 $Pa \cdot s$ to see the sensitivity of the model.

5.2 Comparison of the present 1D model with the 2D model from Rief (2005)

To appraise the quality of the one-dimensional model we compare our numerical results for $\tau = 0$ $Pa \cdot s$ with results obtained in Rief (2005). The model realized in Rief (2005) is two-dimensional and takes into account the geometry of the press rolls. The distribution of pressure obtained by the model from Rief (2005) for the set of parameters described above is presented in Figure 11. Note, that this experiment is possible only in the one layer case. To be able to compare simulation results we average the pressure obtained by 2D model in vertical direction. Pressures are plotted in Figure 12 and the difference between them in Figure 13. From this experiment we can see that the order of the error between the one- and the averaged two-dimensional models is about 1%. The error consists of two parts. The first part arises from omitting the vertical direction. This part of the error is irreducible. The second part appears due to the different approximation schemes. The two dimensional model is discretized by the finite element method. Our numerical scheme is obtained by the finite volume method and the upwind approximation is used to discretize the convective term. Due to this fact in the Figure 12 we observe a shift of the pressure curves, which can be reduced by refining the mesh. Hence, we can conclude that the obtained one-dimensional model suits for the simulation of the pressing section of a paper machine in one layer case and in case of the diagonal intrinsic permeability tensor.

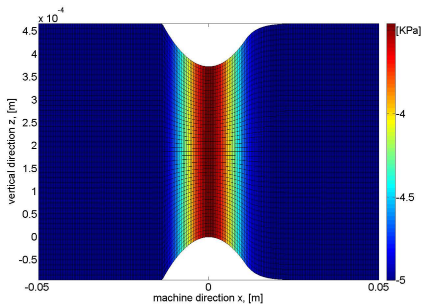

Fig. 11 Distribution of pressure for two-dimensional model

5.3 Convergence test

It is known that in the case of non-smooth data, unphysical effects can be observed in the numerical solution. Therefore, we perform the numerical experiment for different

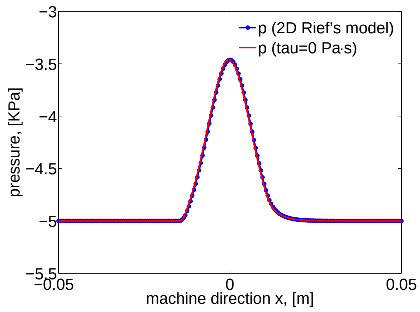

Fig. 12 Comparison of distributions of pressure for one- and two-dimensional models

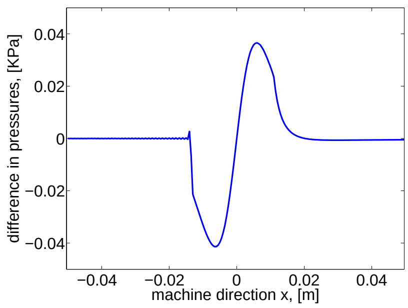

Fig. 13 Difference in pressures for one- and two-dimensional models

types of input data to appraise the rate of convergence of the approximate solution to the continuous one.

Since the analytical solution is unknown, we consider a reference solution with a very small mesh size h^*. This approximation of the continuous solution is defined as p^*. Then, we obtain the dependence of the error E between the discrete solution p^h and the reference solution p^* in the L_2-norm:

$$E(h) = \frac{\|p^* - p^h\|_{L_2}}{\|p^*\|_{L_2}},$$

where h is the size of mesh. We should notice that p^* is not the exact solution therefore if we change h^* the dependence $E(h)$ can also change. But we assume that h^* is small enough so that these changes are not significant.

We consider three different cases for input data, the porosity $\phi(x)$ and the thickness of the layer $d(x)$. The first experiment is carried out for the data which is continuous, but not continuously differentiable, $\phi(x),\ d(x) \in C$. These curves have one point $\hat{x} \in (A, B)$ where first derivatives do not exist. Then, to obtain the second case when the input data is at least twice continuously differentiable, $\phi(x),\ d(x) \in C^2$, we apply the spline interpolation to intervals which contain $\hat{x}$ such that $(\hat{x}-l_i/2, \hat{x}+l_i/2)$ for $i = 1, 2, 3$. These intervals have lengths $l_1 = 2\ mm$, $l_2 = 5\ mm$ and $l_3 = 10\ mm$, respectively. For the third experiment we use such functions for the porosity and the thickness of the layer that they are differentiable for all degrees of differentiation, $\phi(x),\ d(x) \in C^\infty$, and given by:

$$\begin{aligned} \phi(x) &= \frac{\phi_0 - \epsilon(x)}{1 - \epsilon(x)}, \\ d(x) &= d_0(1 - \epsilon(x)), \end{aligned}$$

where $d_0 = 0.56\ mm$ and

$$\epsilon(x) = \frac{C_i}{\sqrt{2\pi 49}} e^{-\frac{x^2}{2\cdot 49}},\ i = 1, 2,$$

with $C_1 = 4.9$ and $C_2 = 5.9$. Thus, we study the convergence in six numerical experiments. Results for the model with the stationary capillary pressure-saturation relation ($\tau = 0\ Pa \cdot s$) are presented in Figure 14. For dynamic capillary pressure with $\tau = 10\ Pa \cdot s$ the convergence results are shown in Figure 15.

For the model with stationary capillary pressure ($\tau = 0\ Pa \cdot s$) (see Figure 14), the rate of convergence is $O(h)$, but the convergence behavior is the same for all types of input data. In case $\tau = 10\ Pa \cdot s$ the convergence rate is also $O(h)$ for all data types.

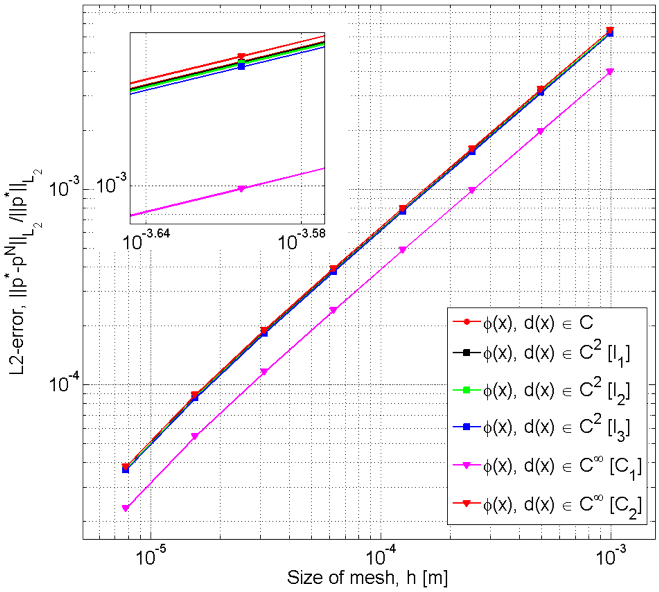

Fig. 14 Convergence results for model (25), (31)-(34) with $\tau = 0\ Pa \cdot s$

6 Conclusion

The first objective of this work was to observe a behaviour of the capillary pressure-saturation relation developed by Hassanizadeh and Gray. This relation has shown a significant influence on the results. The obtained profiles of pressure and saturation affected by the new description of the capillarity have agreed with the physical behavior of the pressing process which was observed in laboratory experiment (Beck, 1983).

The second objective was to develop an accurate one-dimensional model for modeling the pressing section of the paper machine. We have used an averaging procedure to obtain the one-dimensional model which contains information about other directions. This model has given very good results, which are comparable with results obtained by two-dimensional model.

The numerical experiments showed that the material coefficient τ has great influence on the solution. According to the laboratory experiment presented in Beck (1983) we expect that the order of the coefficient τ is $10\, Pa \cdot s$. But there is no

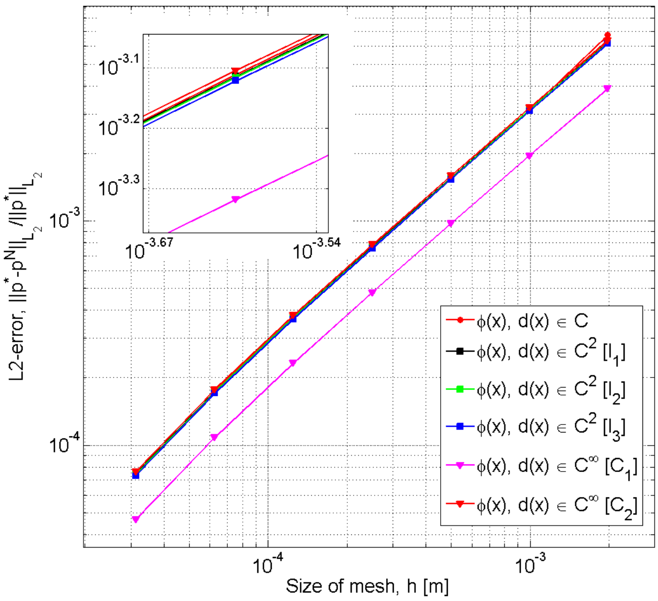

Fig. 15 Convergence results for model (25), (31)-(34) with $\tau = 10\, Pa \cdot s$

information about the range of the coefficient τ for the present problem and more work, including measurements, is needed.

A Second order approximation in case of a standard capillary pressure-saturation relation

As it was mentioned in Remark 1 it is possible to construct the second order finite difference scheme for problem with standard capillary pressure-saturation relation. This case is presented by equations (43)-(46) together with (54)-(56) when the convective term in (25) approximated by central differences. Here we discuss results, which are obtained using this approximation.

Solving system (43)-(46), (54)-(56) by Newton's method the Jacobian $\mathbf{J}_F$ defined by (60) has the following entries:

$$
\begin{aligned}
\frac{\partial F_i}{\partial p_{i-1}} &= d_i \frac{K(\phi_i)}{\mu h}\Big((k_r(\hat{S}_i))'_{p_{i-1}}(p_i - p_{i-1}) - k_r(\hat{S}_i)\Big) \\
&\quad - V_s d_i \phi_i (\hat{S}_i)'_{p_{i-1}}, \quad i = \overline{1, N-1}, \\
\frac{\partial F_i}{\partial p_i} &= -d_{i+1} \frac{K(\phi_{i+1})}{\mu h}\Big((k_r(\hat{S}_{i+1}))'_{p_i}(p_{i+1} - p_i) - k_r(\hat{S}_{i+1})\Big) \\
&\quad + d_i \frac{K(\phi_i)}{\mu h}\Big((k_r(\hat{S}_i))'_{p_i}(p_i - p_{i-1}) + k_r(\hat{S}_i)\Big) \\
&\quad + V_s(d_{i+1}\phi_{i+1}(\hat{S}_{i+1})'_{p_i} - d_i \phi_i (\hat{S}_i)'_{p_i}), \quad i = \overline{1, N-1}, \\
\frac{\partial F_i}{\partial p_{i+1}} &= -d_{i+1} \frac{K(\phi_{i+1})}{\mu h}\Big((k_r(\hat{S}_{i+1}))'_{p_{i+1}}(p_{i+1} - p_i) + k_r(\hat{S}_{i+1})\Big) \\
&\quad + V_s d_{i+1} \phi_{i+1} (\hat{S}_{i+1})'_{p_{i+1}}, \quad i = \overline{1, N-1}, \\
\frac{\partial F_N}{\partial p_{N-1}} &= d_N \frac{K(\phi_N)}{\mu h}\Big((k_r(\hat{S}_N))'_{p_{N-1}}(p_N - p_{N-1}) - k_r(\hat{S}_N)\Big) \\
&\quad - V_s d_N \phi_N (\hat{S}_N)'_{p_{N-1}}, \\
\frac{\partial F_N}{\partial p_N} &= d_N \frac{K(\phi_N)}{\mu h}\Big((k_r(\hat{S}_N))'_{p_N}(p_N - p_{N-1}) + k_r(\hat{S}_N)\Big) \\
&\quad + V_s(d_{N+1}\phi_{N+1}(\hat{S}_{N+1})'_{p_N} - d_N \phi_N (\hat{S}_N)'_{p_N}),
\end{aligned}
$$

Distribution of pressure is shown in Figure 16 for two types of approximation of the saturation (51),(53) and (54)-(56). The numerical solution for (54)-(56) result in nonphysical oscillations close to the points where the input data is not smooth (see Figure 16).

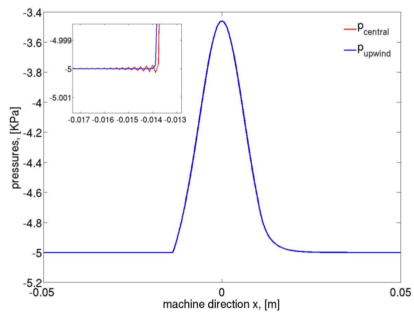

Fig. 16 Distributions of pressure for different approximations of the convective term

We also carry out the convergence test, which shows that the convective term approximated by central differences gives the convergence rate $O(h^2)$ (see Figure 17). From Figure 17 we remark that in this case to obtain the best convergence of the approximate solution to the continuous one it is enough to require continuous second derivatives from the porosity $\phi(x)$ and the thickness of the layer $d(x)$.

Acknowledgements The authors express their deep gratitude to Prof.S.M.Hassanizadeh for the interesting discussions and for his valuable suggestions.

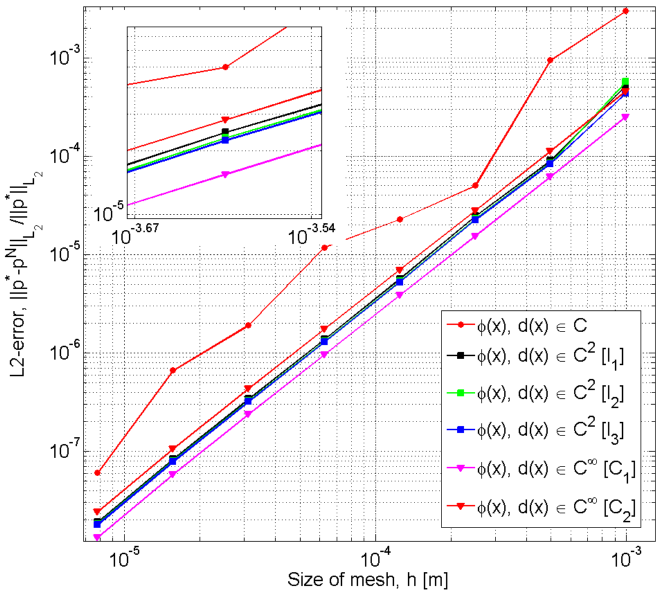

Fig. 17 Convergence results for model (25), (31)-(34) with $\tau = 0\ Pa \cdot s$ and the convective term in (25) approximated by the central differences

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