Modeling of capillary-driven flows in axisymmetric geometries

Citation for published version (APA):

Chassagne, R., Dörfler, F., Guyenot, M., & Harting, J. (2019). Modeling of capillary-driven flows in axisymmetric geometries. *Computers & Fluids*, 178, 132-140. <https://doi.org/10.1016/j.compfluid.2018.08.024>

Document license:
TAVERNE

DOI:
[10.1016/j.compfluid.2018.08.024](https://doi.org/10.1016/j.compfluid.2018.08.024)

Document status and date:
Published: 15/01/2019

Document Version:
Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

[Link to publication](#)

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license above, please follow below link for the End User Agreement:

www.tue.nl/taverne

Take down policy

If you believe that this document breaches copyright please contact us at:

openaccess@tue.nl

providing details and we will investigate your claim.

Modeling of capillary-driven flows in axisymmetric geometries

Romain Chassagne^{a,*}, Fabian Dörfler^a, Michael Guyenot^a, Jens Harting^{b,c}

^a Robert Bosch GmbH, Robert-Bosch-Campus 1, Renningen 71272, Germany

^b Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Strasse 248, Nürnberg 90429, Germany

^c Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, Eindhoven, MB 5600, The Netherlands

ARTICLE INFO

Article history:

Received 20 November 2017

Revised 6 August 2018

Accepted 27 August 2018

Available online 28 August 2018

MSC:

00-01

99-00

Keywords:

Capillary-driven infiltration

Spontaneous imbibition

Free-surface lattice-Boltzmann (FSLB)

ABSTRACT

We present an analytical approach, as well as computer simulations based on the free surface lattice-Boltzmann (FSLB) method, in order to model capillary-driven infiltration of liquids into porous structures. The analytical method is an extension of the Lucas-Washburn (LW) equation and applies to axisymmetric geometries with a circular cross-section. The treatment of irregular capillaries is achieved by a discretization procedure in which the original geometry is divided into small cylinders. In order to validate the derived analytical equation, we perform FSLB simulations in test geometries which show a good agreement.

© 2018 Published by Elsevier Ltd.

1. Introduction

Independently from each other, Lucas [1] and Washburn [2] proposed, respectively in 1918 and 1921, a formula to determine the infiltration rate of liquids into cylindrical capillaries, when only driven by capillary pressure. Due to the simplicity of this equation, it is commonly used beyond its regime of validity, namely to model infiltration processes in porous media by means of some fit parameter, called either “equivalent” or “effective” radius [3]. Even though the infiltration behavior in non-straight geometries is similar to the one in cylinders in that sense that it is also a function of the square root of time, the original LW equation cannot capture the complexity of the effects induced by a cross-section variation. The equivalent capillary model makes, among other things, two incorrect approximations. Firstly, it considers a constant Laplace pressure, whereas the irregularities of a porous medium make it space-dependent. The use of an equivalent radius actually compensates for the geometry irregularities and is only valid for the specific value of the contact angle used for the fit. Consequently, it does not allow to study the effect of a contact angle variation, which would require one fit parameter per contact angle. Secondly, the use of an effective radius can only reproduce one of both characteristics of the flow, in so far as the infiltrated

height of the fluid $h(t)$ and its corresponding infiltrated volume $V(t)$ are, in irregular geometries, not linearly correlated.

Some recent works [4–6] already proposed analytical equations to model infiltration into irregular capillaries composed of basic patterns in which the radius discontinuously varies between two values, also called two-sized single pore model [7]. Among them, Nguyen and Sørensen [5] and Berli et al. [6] use this model as a qualitative explanation to the observed slow infiltration rate in porous media. By contrast, our work aims at developing a simple analytical method that is able to quantitatively describe the infiltration dynamics in more complex axisymmetric capillaries.

The technological background of this work is the diffusion soldering process [8,9] i.e. an alternative soldering technology for semi-conductor devices based on the infiltration of a melted solder alloy into a solid porous matrix of copper. At the pore scale, the influence of gravity becomes negligible such that the infiltration process occurs under capillary forces only. However, the limited application of this technology to small devices hinders its industrial development. A better understanding through an adequate modeling of the infiltration process should permit to optimize it and thus to broaden its field of application.

The remainder of the paper is organized as follows: in Section 2, our analytical approach based on the Hagen–Poiseuille equation and on the mass conservation principle is introduced. Then, in Section 3, a short overview of the free-surface lattice-Boltzmann method (FSLBM) is given. In Section 4 we present our validation and in Section 5 we conclude.

* Corresponding author.

E-mail address: romain.chassagne@de.bosch.com (R. Chassagne).

2. Capillary-driven infiltration processes

2.1. From Hagen–Poiseuille to Lucas–Washburn

The Hagen–Poiseuille equation [10,11] describes pressure-driven, stationary flows of incompressible Newtonian fluids through channels with constant cross-sections. For a cylindrical capillary of length L and radius R , it gives the volumetric flow rate $Q = dV/dt$ as a function of the dynamic viscosity η and of the pressure drop Δp between both capillary ends [12],

$$\frac{dV}{dt} = \frac{\pi R^4 \Delta p}{8\eta L}. \quad (1)$$

In the case of capillary-driven flows, both the inlet and outlet of the geometry are at atmospheric pressure p_0 . The pressure gradient between the capillary entrance and the interface position l which engenders the infiltration results from the local pressure difference Δp at the interface, referred to as Laplace pressure. The latter is caused by the interface curvature and is according to the Young–Laplace equation [13,14] a function of the liquid–gas surface tension σ , the contact angle θ and of the geometry. Within a cylindrical capillary of radius R , the Laplace pressure is uniform and equal to

$$\Delta p = \frac{2\sigma \cos \theta}{R}. \quad (2)$$

Substituting Eq. (2) into Eq. (1) applied between 0 and l and dividing both sides by the cross-sectional area of the capillary $S = \pi R^2$ leads to the Lucas–Washburn equation as defined in [2]

$$\frac{dl}{dt} = \frac{R\sigma \cos \theta}{4\eta l}. \quad (3)$$

Integrating this equation between 0 ($l(0)$ is chosen equal to 0) and a time t at which the interface reaches coordinate l gives

$$l(t) = \sqrt{\frac{R\sigma \cos \theta}{2\eta} t}. \quad (4)$$

In this work, θ refers to the equilibrium contact angle so that the infiltrated length is, in straight capillaries, directly proportional to the square root of time.

2.2. Considering cross-section changes along the infiltration direction

2.2.1. Discontinuous cross-section variations

In this paragraph, the derivation of a LW-like equation for geometries composed of cylinders of different cross-sections is detailed. As for the classical LW equation, inertial effects are not taken into account since they do not play a role for the microscale applications we are interested in. The term “sub-capillary” refers to a part of a capillary in which the cross-section is constant. For the rest of this work, we assume that the flow velocity $\mathbf{u}$ is unidirectional, i.e. that it only has a component u along the infiltration axis x . Besides, for the diverse integral calculations – and except for the Laplace pressure determination – the liquid–gas interface is considered to be flat. The fluid is supposed to move as a block with velocity

$$u_{mean}(x) = \frac{1}{A(x)} \int_0^{2\pi} \int_0^{R(x)} u(x) r dr d\varphi, \quad (5)$$

where $A(x)$ and $R(x)$ are respectively the cross-sectional area and the radius of the capillary at coordinate x . Given that the velocity profile has no consequence on the infiltration behavior, the use of the mean flow velocity $u_{mean}(x)$ in the upcoming equations is a minor approximation which permits to simplify them without violating the principle of mass conservation. Finally, the infiltration is assumed to go on at the intersection of two successive

Fig. 1. Sketch of a capillary of length $3L$ with variable cross-section denoted by radii R_1 , R_2 , R_3 . The liquid penetrates the system at coordinate $x = 0$.

sub-capillaries, i.e. the liquid wets instantaneously the next sub-capillary.

In geometries with variable cross-section, the Laplace pressure Δp is not uniform anymore. As for the derivation of the LW equation, the starting point is the Hagen–Poiseuille equation including now the spatial dependence of the radius. On the infiltration axis, at some coordinate x different from the interface coordinate l , this leads to

$$\frac{dV}{dt} = \frac{\pi R^4(x) dp}{8\eta dx}. \quad (6)$$

Furthermore, the definition of the volumetric flow rate gives [12]

$$\frac{dV}{dt} = A(x) u_{mean}(x) = \pi R^2(x) u_{mean}(x). \quad (7)$$

Combining the previous two equations and integrating from 0 to the interface position l results in

$$\int_0^l \frac{u_{mean}(x)}{R^2(x)} dx = \frac{\Delta p}{8\eta}. \quad (8)$$

As the Laplace pressure corresponds to the pressure difference across the interface, it depends on the capillary radius at the interface position $R(l)$ so that substituting Eq. (2) into (8) leads to

$$R(l) \int_0^l \frac{u_{mean}(x)}{R^2(x)} dx = \frac{\sigma \cos \theta}{4\eta}. \quad (9)$$

The link between the mean flow velocity $u_{mean}(x)$ at $x < l$ in any sub-capillary to the velocity dl/dt of the interface can be found by using the principle of mass conservation [4], according to which

$$u_{mean}(x) A(x) = u_{mean}(l) A(l). \quad (10)$$

As a consequence, the mean velocity at coordinate x can be written as

$$u_{mean}(x) = \frac{dl}{dt} \frac{A(l)}{A(x)}. \quad (11)$$

The expression of $u_{mean}(x)$ from Eq. (11) is then substituted into (9), which results in

$$R^3(l) dl \int_0^l \frac{dx}{R^4(x)} = \frac{\sigma \cos \theta}{4\eta} dt. \quad (12)$$

Finally, to determine the time t_0 at which the liquid–gas interface reaches any coordinate x_0 within the whole capillary, one needs to integrate the above equation between 0 and x_0

$$\int_0^{x_0} R^3(l) \left[\int_0^l \frac{dx}{R^4(x)} \right] dl = \frac{\sigma \cos \theta}{4\eta} t_0. \quad (13)$$

To illustrate the effect of a cross-section change on the infiltration behavior, Eq. (13) is applied to the geometry depicted in Fig. 1 and the resulting infiltration curves are plotted in Fig. 2. The sub-capillary length L is chosen to be constant and equal to $50 \mu\text{m}$. The three radii are defined as $R_1 = 4 \mu\text{m}$, $R_2 = 6 \mu\text{m}$ and $R_3 = 2 \mu\text{m}$. The dynamic viscosity, the contact angle and the surface tension are constant and respectively equal to $\eta = 1.67 \cdot 10^{-10} \text{ Pa}\cdot\text{s}$, $\sigma = 0.05 \text{ N/m}$ and $\theta = 0^\circ$. As already mentioned, the plots of both the infiltrated height of liquid and its associated volume are necessary

Fig. 2. Comparison of the infiltration dynamics in the geometry depicted in Fig. 1 (full lines) and in straight capillaries (dashed lines). Symbols denote a cross-section change.

to describe the effects of a cross-section variation on the infiltration dynamics.

By way of comparison, the infiltration curves for straight capillaries, respectively of radius R_1 and R_3 , are also plotted in Fig. 2. The infiltration in the first sub-capillary is naturally described by the LW equation for a cylinder of radius R_1 . Due to the fact that the volume of the second sub-capillary is larger than the volume of the first one, the average volumetric flow rate in the second sub-capillary increases whereas the interface velocity goes down. More precisely, at the entrance of the second sub-capillary, the flow rate is slightly lower than the one in a straight cylinder of radius R_1 , but the latter decreases faster in the long-term. Conversely, at the entrance of the last sub-capillary, the volumetric flow rate shortly increases before sharply declining. These local effects can be explained by comparing the changes of the viscous and capillary forces [15]. At the entrance of the next sub-capillary, the capillary force, which is proportional to $1/R(l)$, changes suddenly whereas the viscous force, which acts on the total infiltrated liquid, is only slightly affected. More generally, due to the mass conservation principle, a capillary radius reduction results in both a lower flow rate and a lower interface velocity in the long term.

In real geometries, the cross-section changes are barely so sharp. It is thus necessary to extend this model to geometries with a continuously varying radius.

2.2.2. Continuous cross-section variations

In non-straight geometries, the Laplace pressure also depends on the local inclination of the geometry. To be able to treat such cases, as e.g. infiltration into conical capillaries, one has to adapt the expression of the Laplace pressure accordingly which then becomes [16]

$$\Delta p(l) = \frac{2\sigma \cos(\theta + \alpha(l))}{R(l)}, \quad (14)$$

where $\alpha(l)$ accounts for the orientation of the geometry with respect to the infiltration direction at the interface position l . Fig. 3 represents conical capillaries for which the value of α (half the apex angle) is constant. The latter is chosen to be positive for diverging capillaries and negative for converging ones. $\theta_c = 90^\circ - \alpha$ denotes the critical contact angles from which no infiltration occurs. As a consequence, capillary-driven infiltration into converging capillaries can also happen for non-wetting liquids (i.e. $\theta \geq 90^\circ$) whereas wetting liquids do not necessarily infiltrate diverging capillaries. Indeed, the pressure difference across a liquid-gas interface

Fig. 3. Representation of the critical contact angle θ_c in truncated conical capillaries.

results from its curvature, so that it is equal to zero when the interface is flat (i.e. $\theta = \theta_c$) [17]. In that sense, the use of the classical LW equation involving a fit parameter to describe the infiltration dynamics in porous media can lead to erroneous results.

Alternatively, one can adapt Eq. (13) so that it takes this additional geometrical parameter into account

$$\begin{aligned} t_0 &= \int_0^{x_0} \frac{4\eta R^3(l)}{\sigma \cos(\theta + \alpha(l))} \left[\int_0^l \frac{dx}{R^4(x)} \right] dl \\ &= \int_0^{x_0} \lambda(l) R^3(l) \left[\int_0^l \frac{dx}{R^4(x)} \right] dl, \end{aligned} \quad (15)$$

where the parameter $\lambda(l) = \frac{4\eta}{\sigma \cos(\theta + \alpha(l))}$ is introduced for the sake of clarity. In the next paragraph, Eq. (15) is applied to a discretized geometry and a discrete equation is derived.

2.2.3. Discrete infiltration equation

As illustrated in Fig. 4, the proposed discretization procedure consists of dividing an axisymmetric geometry in N small cylinders of constant length L and to apply Eq. (15) to calculate the time necessary to reach the end of each cylinder. Even though the geometry is discretized into straight cylinders, the influence of the local orientation of the geometry is reproduced by the discretized geometrical angle α_i at coordinate $x = (i-1)L$

$$\alpha_i = \arctan \left(\frac{R_{i+1} - R_i}{L} \right), \quad (16)$$

where the index i goes from 1 to N and refers to the number of the cylinder. Consequently, referring to the critical contact angle value, the condition for further infiltration becomes

$$R_{i+1} < R_i + L \tan(90^\circ - \theta). \quad (17)$$

Fig. 4. Discretization of a converging-diverging axisymmetric geometry (full lines) into small straight cylinders of equal length (dashed lines).

Fig. 5. The four different types of cells in a FSLB scheme. Interface cells ($0 < \varphi < \rho$) are first tracked before computing the interface advection.

Eq. (15) is first applied to calculate the time needed for the liquid-gas interface to reach coordinate L . It leads to an equation similar to the LW one, in which λ_1 accounts for the local inclination of the geometry with respect to the infiltration axis

$$t(L) = \frac{\lambda_1 L^2}{2R_1}. \quad (18)$$

Then, calculating the time needed for the full infiltration of the second and third sub-capillaries leads to

$$t(2L) = t(L) + \lambda_2 L^2 \left[\frac{1}{2R_2} + \frac{R_2^3}{R_1^4} \right], \quad (19)$$

$$t(3L) = t(2L) + \lambda_3 L^2 \left[\frac{1}{2R_3} + R_3^3 \left(\frac{1}{R_1^4} + \frac{1}{R_2^4} \right) \right]. \quad (20)$$

More generally, for geometries discretized into N sub-capillaries of equal length, the time needed for the full infiltration of the i th cylinder is given as a recurrence formula

$$\forall i \in [2, N]: \quad t(iL) = t([i-1]L) + \lambda_i L^2 \left[\frac{1}{2R_i} + R_i^3 \sum_{k=1}^{i-1} \frac{1}{R_k^4} \right]. \quad (21)$$

This recurrence formula permits to easily model the infiltration dynamics in complex axisymmetric geometries. Nonetheless, one should keep in mind that the derived equations are a simplified model based on the assumption that the flow is unidirectional. As a result, the larger the angle α , the larger the error (Fig. 5)

3. The free-surface lattice-Boltzmann method (FSLBM)

Free surface flows, i.e. flows in which there is a liquid-gas interface, are present in several industrial applications, as e.g. in oil recovery or injection molding processes [18]. In the considered case of diffusion soldering, the high density difference between the melted solder alloy and the gas atmosphere under which the process takes place renders the dynamics of the gas phase irrelevant. Therefore, the free-surface lattice-Boltzmann method is particularly suitable in such cases in so far as it is a single-phase model in which the gas phase is neglected. Unlike diffuse interface schemes,

the FSLB is a sharp interface model in which the interface has to be tracked and reconstructed [19].

For the simulations in this article we use the software package *Palabos*, which is based on a D3Q19 lattice and a two-relaxation-times scheme. It refers to the classical LB equation [20]

$$f_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) - f_i(\mathbf{x}, t) = C_i(\mathbf{f}(\mathbf{x}, t)), \quad (22)$$

where C_i represents the collision operator. In the LBM, the units are defined through the lattice spacing δx , the time step δt and the unit mass δm [21]. For convenience, we choose to work in lattice units, i.e. $\delta x = \delta t = \delta m = 1$.

In FSLB schemes, the lattice cells are attributed a mass parameter m which can take values between 0 and ρ . The corresponding volume fraction φ at time t is defined as

$$\varphi(\mathbf{x}, t) = m(\mathbf{x}, t) / \rho(\mathbf{x}, t). \quad (23)$$

In this way, it is possible to distinguish the lattice cells in four types: solid, liquid, interface and vacuum [22].

3.1. The interface advection

The advection scheme implemented in *Palabos* is based on the mass exchange principle as in the work of Körner [22]. A volume of fluid approach is used to track each interface cell. The latter exchanges mass with either other interface cells (I) or fluid ones (F) according to

$$\begin{aligned} \delta m_i(\mathbf{x}, t) &= \begin{cases} \frac{\varphi(\mathbf{x}, t) + \varphi(\mathbf{x} + \mathbf{c}_i \delta t, t)}{2} (f_i(\mathbf{x} + \mathbf{c}_i \delta t, t) - f_i(\mathbf{x}, t)) & \text{if } \mathbf{x} + \mathbf{c}_i \delta t \in I, \\ f_i(\mathbf{x} + \mathbf{c}_i \delta t, t) - f_i(\mathbf{x}, t) & \text{if } \mathbf{x} + \mathbf{c}_i \delta t \in F, \end{cases} \end{aligned} \quad (24)$$

where $\bar{i}$ indicates the opposite direction of i . At the next time step, the mass values of the concerned cells are updated following

$$m(\mathbf{x}, t + \delta t) = m(\mathbf{x}, t) + \sum_{i=1}^{19} \delta m_i(\mathbf{x}, t). \quad (25)$$

An interface cell turns into a fluid (gas) one, if $m \geq \rho$ (respectively, $m \leq 0$).

3.2. Reconstruction of unknown distribution functions

Due to the fact that the gas phase is disregarded, the distribution functions that should come from it are unknown and have to be reconstructed. This is done by balancing the forces exerted by the gas and the liquid on the interface [22]. The former is given by the gas pressure and by choosing the gas density ρ^G equal to unity. Besides, the gas phase is assumed to have the same velocity $\mathbf{u}$ as the liquid at the interface. These boundary conditions permit to write the unknown distribution functions as

$$f_i(\mathbf{x} + \mathbf{c}_i \delta t, t) = f_i^{eq}(\rho^G, \mathbf{u}) + f_i^{eq}(\rho^G, \mathbf{u}) - f_i(\mathbf{x}, t), \quad (26)$$

where f_i^{eq} is the equilibrium distribution function associated to $\mathbf{c}_i$ [20]. Considering the local interface normal vector $\mathbf{n}$, all distribution functions which satisfy $\mathbf{n} \cdot \mathbf{c}_i > 0$ are reconstructed. For that purpose, $\mathbf{n}$ is calculated as the gradient of the volume fraction $\mathbf{n} = \nabla \varphi$. For interface cells juxtaposing solid ones, one has to locally modify the normal vector so that it reproduces the contact angle θ given as input parameter [23]

$$\mathbf{n} = \cos \theta \mathbf{n}_{wall} + \sin \theta \mathbf{t}_{wall}. \quad (27)$$

After applying a Laplacian smoothing to the volume fraction, the local interface curvature κ is computed by finite differences using the unit normal vector $\hat{\mathbf{n}}$ [24]

$$\kappa = - \left(\nabla \cdot \frac{\nabla \varphi}{\|\nabla \varphi\|} \right) = - \nabla \cdot \hat{\mathbf{n}}. \quad (28)$$

Finally, the effect of the surface tension in the simulations is reproduced through an additional term — corresponding to the Laplace pressure — in the expression of the gas pressure for interface cells [24]

$$p^G(t) = c_s^2 \rho^G(t) + 2\sigma\kappa(\mathbf{x}, t). \quad (29)$$

Based on comparisons between simulations and analytical results, the next section aims at verifying to what extent Eq. (21) can be applied to describe capillary-driven flows in irregular geometries.

4. Verification and results

In this section, first the configuration used for all performed LB simulations is detailed. Then the ability of the FSLB method to correctly model capillary-driven flows is verified by comparing simulations results in straight cylindrical capillaries to the corresponding LW ones. Finally, the proposed analytical equation for flows in irregular capillaries is verified based on simulation results. Indeed, the derivation of Eq. (15) is based on the assumptions that the flow is uniaxial and that the interface has the form of a spherical cap. The second assumption is no longer valid if the radius of the geometry changes abruptly. As a matter of fact, the interface geometry is also constrained by the capillary shape, i.e. the analytically calculated Laplace pressure from Eq. (14) does no longer match the real one in such cases.

4.1. Configuration of simulations

The general configuration of all performed simulations is identical and is described in this part. All results are given in lattice units (l.u.). In the FSLBM, we define the following parameters as input: the fluid density ρ and the kinematic viscosity ν , the liquid-gas surface tension σ , the equilibrium contact angle θ as well as the inlet and ambient pressures p_{inlet} and $p_{ambient}$. The relaxation time τ is chosen equal to 1, which constraints the kinematic viscosity value to $1/6$ [20,25]. Consequently, changes in the dynamic viscosity $\eta = \rho\nu$ are obtained by a variation of the fluid density. There is no pre-infiltrated liquid in the geometry at time 0 and no external force has been defined. In order to reproduce capillary-driven infiltration processes, both inlet ($x = 0$) and ambient pressures are set to zero. In that way, the only pressure difference is the Laplace pressure Δp across the liquid-gas interface. This boundary condition amounts to set the LB density at the inlet equal to 1 according to [24]

$$\rho_{inlet}^{LB} = \frac{1}{\rho c_s^2} \frac{\delta t^2}{\delta x^2} (p_{inlet} - p_{ambient}) + \rho^{LB} = 1. \quad (30)$$

Mid-grid bounce-back boundary conditions are applied at solid nodes, resulting in the actual liquid-solid boundary to be situated between two neighbor solid and liquid nodes. As a consequence, the effective radius of the capillary is reduced by approximately half a lattice interval as compared to the value given as input for the simulations [26]. This effect is taken into account through a constant modification of the radius when comparing simulations and analytical results.

4.2. Infiltration into cylindrical capillaries

The ability of the FSLBM to correctly reproduce capillary-driven infiltration processes is first investigated. The verification is based on a comparison of simulation results for flows in cylindrical capillaries with the results of the LW equation. The main parameters playing a role in capillary-driven processes are varied one by one: the fluid dynamic viscosity η , the liquid-gas surface tension σ and the contact angle θ . In the first instance, a capillary of length 200 in the infiltration direction and of fixed radius R equal to 10 is

Fig. 6. Capillary-driven infiltration of a liquid into a straight capillary of radius 10.

Fig. 7. Comparison of analytical and simulated infiltration dynamics in a capillary of radius 10 for different contact angles.

used, as illustrated in Fig. 6. The results of the simulations are represented via colored markers and compared to the corresponding analytical solutions, represented by continuous black curves depicting the infiltrated height of liquid as a function of the time.

Firstly, the simulation results for a contact angle variation ($\theta = 0^\circ, 40^\circ, 60^\circ, 80^\circ$) at constant viscosity and surface tension are plotted in Fig. 7. In all four cases — which virtually cover the whole range of wetting contact angles — the expected infiltration dynamics is well reproduced. It highlights capacity of the method to deal with a wide range of wetting contact angles, including small ones as, e.g. $\theta = 0^\circ$.

Secondly, the dynamic viscosity and surface tension are varied within one order of magnitude with inversely proportional factors. The reference viscosity ($\eta = 1/6$) is multiplied by 2, 5 and 10 in the left graph of Fig. 8 (at constant surface tension $\sigma = 0.05$ and contact angle $\theta = 0^\circ$), while the surface tension is divided by these same factors in the second graph (at constant viscosity $\eta = 1/6$ and contact angle $\theta = 0^\circ$). Also in these cases, one can observe that the simulated infiltration behavior matches the analytical one. Furthermore, as expected from Eq. (4), the defined variations of η and σ are equivalent.

The presented results validate that the FSLB scheme implemented in Palabos is able to precisely reproduce the influence of each key parameter during capillary-driven infiltration processes. Moreover, additional simulations performed in capillaries with a lower radius resolution show that results of equivalent quality can be achieved for a radius discretized with only 3 lattice spacings.

The next section relies on this proof of concept for the FSLBM and verifies the validity of Eq. (15) for flows in irregular capillaries. The geometries are chosen in such a way that the results of simulations can be compared to the analytics, in spite of the geometry discretization inherent to the LBM.

Fig. 8. Comparison of analytical and simulated infiltration dynamics in a capillary of radius 10 for different viscosities and surface tensions.

Fig. 9. Capillary-driven infiltration of a liquid into capillaries with stepwise changing radii between 5 and 10.

Fig. 10. Comparison of the geometry from the simulations to the corresponding analytical geometries for two different discretization steps L (Eq. (21)).

4.3. Infiltration in capillaries with cross-section changes

4.3.1. Capillaries with a stepwise changing cross-section

This paragraph refers to capillaries with a stepwise changing cross-section as defined in Section 2.2.1. In the first instance, two systems composed of six cylinders, each of length 50, but with different radii are studied (see Fig. 9). The radius of the first geometry is getting larger along the infiltration direction, going from 5 at the entrance of the geometry to 10 at its end whereas the second geometry has a stepwise decreasing radius going from 10 to 5.

The simulation results for different contact angle values are plotted in Fig. 11 and compared to the ones obtained with Eq. (21) using a discretization step $L = 0.1$. Choosing $L = 0.1$ for the analytical geometry permits to smooth the staircase effect at cross-section changes in comparison to $L = 1$ as depicted in Fig. 10. Moreover, it has been verified that further reducing L under 0.1 has a negligible influence on the infiltration dynamics in all studied cases.

For the capillary with growing radius along the infiltration direction, one can observe small plateaus in the simulated infiltration curve $h(t)$ at each cross-section change. The latter are getting larger with higher contact angles. This phenomenon is attributed

to the positions of the bounce-back nodes in the case of small steps along the infiltration direction. As a consequence, the actual geometry, which is basically defined by the position of the bounce-back nodes, does not have a staircase shape but has locally a conical form (due to its axisymmetry) with a continuously increasing radius.

With the aim of using the same geometry for the analytical equation as the one defined in the simulations, it is chosen to reproduce this simulative effect in Eq. (21) through the local use of a geometrical angle $\alpha = +45^\circ$ at each radius change. Conversely, the effect of a radius reduction of 1 has the effect of a wall inclined at -45° (Fig. 14).

Also in these more complex geometries, both analytical and simulated models are in agreement. This indicates that Eq. (21) is able to capture the effects of a cross-section change on the infiltration behavior. As explained in Section 2.2.1, due to mass conservation considerations, the geometry beginning with the narrowest capillary needs much more time than the second one to be fully infiltrated. Next, the infiltration dynamics in a diverging capillary is investigated.

4.3.2. Capillaries with continuously changing cross-section

The used geometry, as depicted in Fig. 12, constitutes of a straight cylinder followed by a diverging capillary. Due to the fact that the slope of the diverging part of the capillary is constant — steps of 1×1 — the bounce-back nodes are aligned, which implies that the LB staircase geometry can be analytically treated as a wall with a constant inclination $\alpha = 45^\circ$ with respect to the horizontal direction.

After the fast infiltration of the straight cylinder at the beginning of the geometry, the infiltration rate significantly decreases in the diverging part. This is due to the sudden fall of the Laplace pressure according to Eq. (14) and to the steadily increasing volume corresponding to a further infiltration of 1. The simulated infiltration curves are plotted in Fig. 13, along with the corresponding results from Eq. (21) using a discretization step $L = 0.1$. To highlight the importance of considering the cross-section changes in Eq. (21), results in which the parameter α has been disregarded are plotted in dashed lines in the left graph. It illustrates the error introduced when modeling porous media with cylindrical capillaries. The relative gaps between the curves are not well reproduced and the use of an equivalent radius does not permit to overcome this model limitation. On the contrary, and even though the flow

Fig. 11. Comparison of analytical and simulated infiltration dynamics in irregular capillaries for different contact angles.

Fig. 12. (a) Capillary-driven infiltration of a liquid into a diverging capillary; (b) Slice of the system along the infiltration direction.

is no longer uniaxial, the complete Eq. (21) is able to reproduce qualitatively, as well as quantitatively, the infiltration dynamics in capillaries with a pronounced radius variation.

4.3.3. Sinusoidal capillary

As a last step to verify the ability of Eq. (21) to model capillary-driven flows in porous axisymmetric geometries, the infiltration into sinusoidal capillaries is investigated. First, three geometries of equal length are considered. The minimal radius R_1 of each is fixed to 3 and the maximal radii R_2 are respectively equal to 8, 13 and 18. Second, the contact angle is varied between 0 and 35° for the geometry of radius $R_2 = 13$. The corresponding analytical and simulated results are plotted in Fig. 15. As before, the discretization step along the infiltration direction used in Eq. (21) is $L = 0.1$.

Fig. 14. (a) Capillary-driven infiltration of a liquid into a sinusoidal capillary ($R_2 = 18$); (b) Slice of the system along the infiltration direction.

Fig. 13. Comparison of analytical and simulated infiltration dynamics in a diverging capillary for different contact angles. The dashed lines correspond to Eq. (21) without taking the geometrical angle α into account.

The observed leaps in the simulated infiltration curves for the largest two geometries are discretization effects which appear at the transition from diverging to converging parts. Indeed, due to the regular grid definition, the LB geometry is not strictly axisymmetric. As a result the liquid phase advances locally faster than the rest of the interface. However, this effect only occurs at the solid-liquid boundary and barely affects the interface curvature – as it

Fig. 15. Comparison of analytical and simulated infiltration dynamics in sinusoidal capillaries for different geometries and contact angles.

can be observed from the free surface geometry – and thus the calculation of the Laplace pressure.

For both parameter variations, the correlation between analytical curves and the ones obtained from simulations is remarkably good. The analytical model does not only correctly predict the full infiltration time for the whole geometry, but it is also able to capture precisely the local accelerations and decelerations of the liquid phase in the different parts of the geometry.

5. Conclusion

We presented an approach aiming at a detailed understanding of capillary infiltration in porous media by combining fully resolved computer simulations of multiphase flow in complex geometries with a simplified analytical approach to describe the infiltration on large scales. While the fully resolved simulations based on the free surface lattice Boltzmann method allow arbitrary geometries and can easily be extended towards inhomogeneous wetting and surface properties, they do not allow to reach macroscale system sizes of technical relevance while still resolving the individual pores at the microscale. Therefore, in this paper we used them to benchmark and validate our simplified analytical approach based on the axisymmetric Lucas-Washburn equation. While the Lucas-Washburn equation only holds for straight cylindrical geometries, we demonstrated that irregular capillaries can be treated by a discretization procedure in which the original geometry is divided into small cylinders. In order to validate the derived analytical equation, we performed FSLB simulations in test geometries which show a good agreement. The aim of our work is to demonstrate that our simplified approach can be of use where the detailed microscopic information including fully resolved flow fields on the pore scale is not necessary, but instead a fast and easy to apply realistic estimate of the macroscale behaviour is desired.

Acknowledgments

The authors are grateful to the FlowKit team for providing the code Palabos and for the helpful discussions.

References

- [1] Lucas R. Ueber das zeitgesetz des kapillaren aufstiegs von flüssigkeiten. *Kolloid-Zeitschrift* 1918;23:15–22. doi:10.1007/bf01461107.
- [2] Washburn EW. The dynamics of capillary flow. *Phys Rev* 1963;17(3):273–83. doi:10.1103/PhysRev.17.273.
- [3] Kalogianni EP, Savopoulos T, Karapantsios TD, Raphaelides SN. A dynamic wicking technique for determining the effective pore radius of pregelatinized starch sheets. *Colloids Surf B, Biointerf* 2004;35(3–4):159–67. doi:10.1016/j.colsurfb.2004.03.008.
- [4] Young W. Analysis of capillary flows in non-uniform cross-sectional capillaries. *Colloids Surfaces A, Physicochem Eng Aspects* 2004;234(1–3):123–8. doi:10.1016/j.colsurfa.2003.12.007.
- [5] Nguyen HT, Sørensen BR. Analytical model of capillary suction velocity of a pipe with multiple sizes. *Adv Mat Res* 2013;652–654:1201–8. doi:10.4028/www.scientific.net/AMR.652-654.1201.
- [6] Berli CLA, Mercuri M, Bellino MG. Modeling the abnormally slow infiltration rate in mesoporous films. *Phys Chem Chem Phys* 2017;19(3):1731–4. doi:10.1039/C6CP06602J.
- [7] Einset EO. Capillary infiltration rates into porous media with applications to silcomp processing. *J Am Ceram Soc* 1996;79(2):333–8. doi:10.1111/j.1151-2916.1996.tb08125.x.
- [8] Herberholz T. Untersuchungen zu Möglichkeiten und Grenzen des Einsatzes von Zinn-Basislotlegierungen für Hochtemperaturelektronikanwendungen. Universität Rostock; 2015.
- [9] Nowotnick M, Pape U, Wilde J. Neue reflowloettechnologie für elektronische anwendungen bis 300C - 'hotpowCon'. *Templin : Detert*; 2015.
- [10] Hagen G. Ueber die bewegung des wassers in engen cylindrischen röhren. *Ann Phys* 1839;122(3):423–42. doi:10.1002/andp.18391220304.
- [11] Poiseuille JLM. Recherches expérimentales sur le mouvement des liquides dans les tubes de très petits diamètres. *Comptes rendus des séances de l'Académie des Sciences* 1840;11:1041–8.
- [12] Bruus H. *Theoretical microfluidics*. Oxford University Press; 2008.
- [13] Young T. III. An essay on the cohesion of fluids. *Phil Trans R Soc Lond* 1805;95:65–87. doi:10.1098/rstl.1805.0005.
- [14] Laplace PS. *Supplément à la théorie de l'action capillaire. traité de mécanique céleste. suppliment 2. livre x, 4. Paris: Gauthier-Villars; 1806.*
- [15] Erickson D, Li D, Park CB. Numerical simulations of capillary-driven flows in nonuniform cross-sectional capillaries. *J Colloid Interface Sci* 2002;250:422–30. doi:10.1006/jcis.2002.8361.
- [16] Dullien FAL. *Porous media: fluid transport and pore structure*. Academic Press; 2012.
- [17] Yang XF, Xi XM. Critical wetting angle for spontaneous liquid infiltration into orderly packed fibres or spheres. *J Mater Sci* 1995;30(20):5099–102. doi:10.1007/BF00356055.
- [18] Vafai K. *Handbook of porous media, third edition*. CRC Press; 2015.
- [19] Liu H, Kang Q, Leonardi CR, Schmieschek S, Narváez A, Jones BD, Williams JR, Valocchi AJ, Harting J. Multiphase lattice boltzmann simulations for porous media applications - a review. *Comput Geosci* 2016;20(4):777–805. doi:10.1007/s10596-015-9542-3.
- [20] Succi S. *The lattice boltzmann equation for fluid dynamics and beyond*. Clarendon Press; 2001.
- [21] Thies M. *Lattice Boltzmann modeling with free surfaces applied to formation of metal foams*. Universität Erlangen-Nürnberg; 2005. Ph.D. Thesis.
- [22] Körner C, Thies M, Hofmann T, Thürey N, Rüde U. Lattice boltzmann model for free surface flow for modeling foaming. *J Stat Phys* 2005;121(1/2):179–96. doi:10.1007/s10955-005-8879-8.
- [23] Bogner S. *Direct numerical simulation of liquid-gas-solid flows based on the lattice Boltzmann method*. Universität Erlangen-Nürnberg; 2017. Ph.D. Thesis.
- [24] FlowKit. Palabos. <http://www.palabos.org/>.

- [25] Krüger T, Kusumaatmaja H, Kuzmin A, Shardt O, Silva G, Viggen EM. The lattice Boltzmann method. Springer International Publishing; 2017. doi:[10.1007/978-3-319-44649-3](https://doi.org/10.1007/978-3-319-44649-3).
- [26] Bogner S, Rüde U, Harting J. Curvature estimation from a volume-of-fluid indicator function for the simulation of surface tension and wetting with a free-surface lattice boltzmann method. Phys Rev E 2016;93(4). doi:[10.1103/PhysRevE.93.043302](https://doi.org/10.1103/PhysRevE.93.043302).