ON NUMERICAL APPROXIMATION OF TWO-PHASE FLOW WITH SURFACE TENSION AND CONTACT ANGLES WITH LEVEL SET APPROACH

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Abstract

In this paper the problem of flow of two immiscible incompressible fluids is considered, mathematically modelled and numerically approximated. The surface tension and the static contact angle effects are considered, its mathematical realization is discussed and applicable numerical procedures are described. The finite element method is used for approximation, the extended finite element method is used to treat the pressure discontinuity caused by the surface tension. The numerical results are shown.

Keywords: finite element method, level set, free surface.

1 Introduction

The numerical simulations become to be very popular in many technical fields in particular they are used for simulation of free surface flows at various scientific as well as technical problems, see e.g. [7], [14], [8], [13], [2]. Particularly also the numerical simulation of two phase flow problem is being used to address various problem from technical practice, [19]. The numerical methods are used for approximation of free surface flows of water, various industrial fluids, molten steel, molten glass at various applications, cf. [9].

In this paper a simplified problem of flow of molten glass is considered particularly during the float process. Although glass as material exists for millions of years, it is still very interesting from both the technological and scientific reasons. At sufficiently high temperatures the (molten) glass behaves like a liquid. By cooling down its viscosity continuously becomes very high and the glass freezes to a solid-like state. This phenomena is used partially during the glass production processes, see [6].

Glass furnaces are used for melting the raw material particles and for transforming these into molten glass. This hot glass material (approximately at 1100-1500 degrees of Celsia) is then used in the glass production, see [6]. Let us consider the fabrication of a flat glass produced nowadays by the float process as introduced by Pilkington in the 1950s, see [18]. Firstly, the raw material given to the furnace is melted at 1500 degrees of Celsia, homogenized by convection and fined to eliminate bubbles. The viscous liquid then moves out of the melting furnace through the part called lip onto the surface of an enclosed bath made of tin. This continuous ribbon of glass is held at a high enough temperature to melt our irregularities and to make its surface perfectly flat. By cooling down of the glass with still advancing through the rollers marking the bottom surface the uniform uniform thickness flat glass is produced. Such a problem is interesting not only for the technical application but also from the mathematical modelling point of view. Particularly the free surface flow of molten glass needs to be addressed. One of the possible approaches is to use a single phase flow with a free surface or the other is the use of a two-phase flow model with the second fluid being the surrounding atmosphere (as e.g. air).

However, the description of a two-phase flow model can be rather difficult as it includes wide variate of fluids (water, oil, industrial materials) with different densities, various viscosities and also with possibly non-Newtonian behaviour. Such flows are moreover usually strongly influenced by the gravitational force and in many cases also the turbulence character of the flow needs to be treated, cf. [5]. Any used mathematical model have to naturally address at least the significant phenomena if not all of these characterizations. As for molten glass flow is concerned the surface tension effects and the static contact angle can play significant role here, and should be taken into account.
Once a mathematical model is formed, it usually needs to be approximated numerically. For the numerical approximation of two-phase flows in complicated geometries either finite volume method or the finite element method can be used. In order to address the free surface motion several available technique as volume of fluid (VOF), level-set (LS) method or arbitrary Lagrangian Eulerian(ALE) like methods can be applied. The resulting mathematical model then needs to be numerically approximated, see among others [3], [10] or [11]. The surface tension effects then can be approximated using the explicit formula, [17]. The other possibility is the use of weak re-formulation with the use of the Laplace-Beltrami operator, see [4], [11]. In this case the main advantage is the possibility to time discretize the surface tension terms implicitly, which increases the stability of the scheme.

In this paper, we consider the two-dimensional flow of two immiscible fluids, the problem is mathematically described and the variational formulation is introduced. For the discretization the finite element(FE) method is used. The free surface motion is realized using the level set method, cf. [17] or [15]. In the case of high surface tension, a modification of the standard FE method is required to avoid the spurious currents, see [16] or [3]. For the verification of the implemented method a benchmark problem is solved, cf. [11].

2 Mathematical models

Variable density flow model. First, we describe a mathematical model of flow of two immiscible fluids (denoted A and B) in a two-dimensional domain $\Omega \subset \mathbb{R}^2$ with Lipschitz continuous boundary $\partial \Omega$. The boundary $\partial \Omega$ consists of mutually disjoint parts $\Gamma_W$ representing the fixed walls, $\Gamma_O$ representing the outlet, $\Gamma_S$ representing wall with slip boundary conditions and (possibly) $\Gamma_I$ representing the inlet. The domain is at any time instant $t$ assumed to be divided into two subdomains $\Omega^A(t)$ and $\Omega^B(t)$ occupied by the fluid A and B, respectively. The mutual boundary of $\Omega^A(t)$ and $\Omega^B(t)$, i.e. the free surface interface, is denoted by $\hat{\Gamma}_t = \overline{\Omega^A(t)} \cap \overline{\Omega^B(t)}$. On $\hat{\Gamma}_t$ the surface tension forces are applied. The fluids A and B are characterized by their densities denoted by $\rho^A$ and $\rho^B$, and also their viscosities $\mu^A$ and $\mu^B$, respectively. In general we consider these values to be constant although these quantities are in general non-constant (e.g. temperature dependent, or e.g. non-linearly dependent on rate of deformation for non-Newtonian fluids).

The flow of the two fluids is mathematically described with the aid of the Heaviside function $H(x, t)$, which satisfies $H(x, t) = 1$ for $x \in \Omega^A(t)$, $H(x, t) = \frac{1}{2}$ for $x \in \hat{\Gamma}_t$ and $H(x, t) = 0$ otherwise. Using the Heaviside function, the variable density $\rho(x, t)$ and viscosity $\mu(x, t)$ formulation can be used, where these functions at a point $x \in \Omega$ at time $t \in (0, T)$ read

$$\rho(x, t) = \rho^A H(x, t) + (1 - H(x, t)) \rho^B,$$  
$$\mu(x, t) = \mu^A H(x, t) + (1 - H(x, t)) \mu^B. \quad (1)$$

The pressure and the flow velocity functions are denoted by $p(x, t)$ and $u = u(x, t)$, respectively. These functions are defined in the whole computational domain $\Omega$, where in $\Omega^A$ these corresponds to pressure and velocity of the fluid A and similarly in $\Omega^B$ these stands for pressure and velocity of the fluid B. As both fluids are considered to be viscous, the velocity field have to be continuous also over the interface $\Gamma_{W,t}$, whereas the pressure field does not have to be continuous here due to the surface tension present. The pressure field in the weak formulation for incompressible fluid is anyway sought in the space $L_2(\Omega)$, where the discontinuous pressures are allowed.

Using this notation the flow motion can be formally described by the variable density formulation of the incompressible Navier-Stokes equations

$$\begin{equation}
\partial_t u + \frac{1}{\rho} \nabla p + \rho (u \cdot \nabla) u - \nabla \cdot \sigma = \rho f + \gamma \kappa n \delta_{\hat{\Gamma}_t},
\end{equation}$$

where $\sigma$ is the Cauchy stress tensor given by

$$\sigma = -p I + \mu (\nabla u + (\nabla u)^T),$$

and $\delta_{\hat{\Gamma}_t}$ is the Dirac delta function of the interface $\hat{\Gamma}_t$, $\gamma$ is the surface tension coefficient, $\kappa$ is the local curvature of the interface and $n$ is the unit normal vector to the interface $\hat{\Gamma}_t$ (oriented into
The Dirac delta functions makes the formulation valid only in its integral form, i.e. for any \( \mathbf{v} \in V \subset H^1(\Omega) \) being at time instant \( t \) it should hold
\[
\int_\Omega \rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) \cdot \mathbf{v} + \mathbf{\sigma} \cdot (\nabla \mathbf{v}) \, dx = \int_{\hat{\Gamma}_t} \gamma \kappa \mathbf{n} \cdot \mathbf{v} \, dS + \int_\Omega \rho \mathbf{f} \cdot \mathbf{v} \, dx. \tag{3}
\]
Here, \( H^1(\Omega) \) is the Sobolev’s space of vector functions with their components being square integrable together with their first derivatives, see [1], and the subspace \( V \) is formed from functions from \( H^1(\Omega) \) being zero on \( \Gamma_W \cup \Gamma_I \) and with zero normal components on \( \Gamma_S \), i.e.
\[
V = \{ \varphi \in H^1 : \varphi = 0 \text{ on } \Gamma_W \cup \Gamma_I, \varphi \cdot \mathbf{n} = 0 \text{ on } \Gamma_S \}.
\]

Further, system of Eqs. (2) is equipped with an initial condition \( \mathbf{u} = 0 \) and for the initial value of the Heaviside function \( H(x,0) = H_0(x) \). The second condition means that the initial location of the two fluids A and B is known (i.e. the domains \( \Omega_A^{(0)} \) and \( \Omega_B^{(0)} \) are specified). Further, on the boundary \( \partial \Omega \) the following boundary conditions are prescribed
\[
a) \quad \mathbf{u} = \mathbf{u}_I \quad \text{on } \Gamma_I, \\
b) \quad \mathbf{u} = 0 \quad \text{on } \Gamma_W, \\
c) \quad \mathbf{u} \cdot \mathbf{n} = 0, \quad t \cdot (\mathbf{\sigma} \cdot \mathbf{n}) = 0 \quad \text{on } \Gamma_S, \\
d) \quad \mathbf{\sigma} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_O. \tag{4}
\]

In order to Eqs. (2), the motion of the computational domains \( \Omega_A^{(t)} \) and \( \Omega_B^{(t)} \) needs to be solved including the motion of the interface \( \hat{\Gamma}_t \). This motion can be formally expressed as the mass conservation law (the continuity equation). Using the continuity equation with the variable density dependent on the Heaviside function, the motion of the interface can be described formally using the equation
\[
\frac{\partial H}{\partial t} + \mathbf{u} \cdot \nabla H = 0, \tag{5}
\]
where \( \nabla \cdot \mathbf{u} = 0 \) as \( \mathbf{u} \) is expected to be solution of (2).

**Level set equation.** Furthermore, to treat the motion of the free surface \( \hat{\Gamma}_t \) the level set method is applied, which means that we solve another equation for the level set function. The level set function is basically the signed distance function being zero on the interface \( \hat{\Gamma}_t \) at any time instant \( t \), positive in \( \Omega_A^{(t)} \) and negative in \( \Omega_B^{(t)} \). The Heaviside function \( H(x,t) \) is then re-defined using the sign of the level set function \( \phi(x,t) \), i.e.
\[
H(x,t) = \begin{cases} 
1 & \text{for } \phi(x,t) > 0, \\
\frac{1}{2} & \text{for } \phi(x,t) = 0, \\
0 & \text{for } \phi(x,t) < 0. 
\end{cases}
\]
The initial condition for the level set function \( \phi \) is given as the signed distance function from \( \hat{\Gamma}_0 \). The motion of the interface \( \hat{\Gamma}_t \) is then realized by solving the transport equation for the function \( \phi(x,t) \), i.e.
\[
\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0, \tag{6}
\]
which guarantees that the interface is moving with the velocity \( \mathbf{u} \).

**Surface tension.** In order to treat the surface tension term, we start with its weak reformulation. Let us define the tangent derivative \( \nabla_\Gamma \) as \( \nabla_\Gamma \mathbf{g} = \nabla \mathbf{g} - (\mathbf{n} \cdot \nabla \mathbf{g}) \mathbf{n} \) and the Laplace-Beltrami operator \( \Delta_\Gamma = \nabla_\Gamma \cdot \nabla_\Gamma \). Now, using the relation \( \kappa \mathbf{n} = \Delta_\Gamma \mathbf{x} \) and applying the integration by parts on \( \hat{\Gamma}_t \) we get
\[
\int_{\hat{\Gamma}_t} \gamma \kappa \mathbf{n} \cdot \mathbf{v} \, dS = \int_{\hat{\Gamma}_t} \gamma (\nabla_\Gamma \mathbf{x}) \cdot \mathbf{v} - \int_{\hat{\Gamma}_t} \gamma (\nabla_\Gamma \mathbf{x}) \cdot (\nabla_\Gamma \mathbf{v}) \, dS, \tag{7}
\]
where on the right hand side the integral over \( \partial \hat{\Gamma}_t \) denotes the integral over the contact lines. For the considered two dimensional case this integral is only sum over the contact points. Under the assumption that \( \hat{\Gamma}_t \) is a closed curve, i.e. no contact of the free surface with the wall occurs, this term equals zero.
3 Numerical approximation

Flow step. For simplicity, let us consider the equidistant partition of the time interval $[0, T)$ given by $t_n = n \Delta t$, where $n = 0, 1, \ldots, N$ and $\Delta t = T/N$. Let us denote by $u^{(n)}$, $p^{(n)}$, $\phi^{(n)}$, $\rho^{(n)}$ and $\mu^{(n)}$ approximations of the velocity, the pressure the level set function, the density and the viscosity at the time instant $t_n$, respectively. Let us approximate the time derivative by the backward Euler formula, i.e.

$$
\frac{\partial u}{\partial t}|_{t=t_n} \approx \frac{u^{(n+1)} - u^{(n)}}{\Delta t}, \quad \frac{\partial \phi}{\partial t}|_{t=t_n} \approx \frac{\phi^{(n+1)} - \phi^{(n)}}{\Delta t}.
$$

Let us assume that $u^{(n)}$, $p^{(n)}$, $\phi^{(n)}$, $\rho^{(n+1)}$ and $\mu^{(n+1)}$ are already known. Then the time discretized weak formulation of Eq. 2 reads: Find $u^{n+1} \in V$ and $p^{n+1} \in Q$ such that

$$
\int_{\Omega} \rho^{n+1}(x) \left( \frac{u - u^n}{\Delta t} + (u \cdot \nabla) u \right) \cdot v - p(\nabla \cdot v) + \mu^{n+1}(x) \nabla u \cdot \nabla v \, dx 
$$

$$
+ \int_{\Omega} (\nabla \cdot u) q \, dx = - \int_{\Gamma^{n+1}} \gamma(\nabla_{\Gamma} x) \cdot (\nabla_{\Gamma} v) \, dS + \int_{\Omega} \rho^{n+1}(x) f \cdot v \, dx \tag{8}
$$

holds for all $v \in V$ and $q \in Q$. In the practical computations we assume that the domain $\Omega$ is a polygonal and the spaces $V$ and $Q$ are approximated by the FE subspaces $V_h$ and $Q_h$ defined over an admissible triangulation $T_h$, respectively. For the approximation the well-known Taylor-Hood FE are used, i.e. the velocity is sought in the space $V_h = [H_h]^2 \subset V$, where $\Omega = [H_h]^2 \subset V$, where $H_h = \{ \phi \in C(\overline{\Omega}); \phi|_K \in P_2(K) \text{ for each } K \in T_h \}$,

$$
H_h = \{ \phi \in C(\overline{\Omega}); \phi|_K \in P_2(K) \text{ for each } K \in T_h \}. \tag{9}
$$

The discrete flow problem then reads: Find $u_h^{n+1} = u^{n+1} \in V_h$ and $p_h^{n+1} = p^{n+1}$ such that Eq. 8 holds for any test function $v := v_h \in V_h$ and $q := q_h \in Q_h$. In order to treat the discontinuity of the pressure due to the presence of the surface tension the extended finite element method (XFEM) is applied, see e.g. [16].

Extended finite element method. Due to the surface tension, the discontinuous pressure across the interface needs to be treated, which possibly can lead to spurious currents appearing at the interface in the case of used continuous finite element pressure space $Q_h$. The XFEM enriches the original FE space $Q_h$ using the localization of an enrichment function. For the localization the original base functions of $Q_h$ are used, i.e. we denote the index set $J = \{ 1, \ldots, n \}$, $n = \dim Q_h$ and the mesh nodes by $x_j$, $j \in J$. The nodal base functions are then denoted by $q_i \in Q_h$, $i \in J$ and satisfy $q_i(x_j) = \delta_{ij}$. The $J'$ is the subset of all the neighbours of the interface $\Gamma$, i.e. $J' = \{ j \in J : \text{supp } q_j \cap \Gamma \neq \emptyset \}$. We shall use the discontinuous enrichment function $H_{\Gamma}(x)$ given as the Heaviside function $H_{\Gamma}(x) = H(x, t_{n+1})$. Now, the enrichment of the space $Q_h$ is made using the discontinuous base functions $q_j^{xfc}$ defined by

$$
q_j^{xfc}(x) = q_j(x) (H_{\Gamma}(x) - H_{\Gamma}(x_j)) \tag{11}
$$

where the term $-q_j(x)H_{\Gamma}(x_j)$ makes the support of the function $q_j^{xfc}(x)$ localized to the single element containing the interface. The FE space $Q_h$ is then replaced by the extended FE space $Q_h^{xfc} = Q_h \oplus \text{span} \{ q_j^{xfc} : j \in J' \}$.

Level set step and coupled problem. Eq. 6 is time discretized, weakly formulated and the standard Galerkin FE method is employed. In order to obtain a stable scheme, the algebraic flux corrections can be applied, see [12]. Nevertheless, in the considered case of a continuous level set function $\phi$, this is mostly equivalent to the Galerkin method (at least for a limited time period). It is also known, that for the level set method a re-initialization step is needed to maintain the distance like property, see also [11]. Thus we simply use the Galerkin FE approximations and perform the re-initialization step every 5-40 iterations. The solution of the coupled problem is then performed by a de-coupled algorithm, where we start with the level set step followed by the solution of Eqs. 8 for approximation of the flow velocity $u^{n+1}$ and the pressure $p^{n+1}$. 


Table 1: The quantitative results for the rising bubble case I: the comparison of the computed and the reference quantities.

<table>
<thead>
<tr>
<th></th>
<th>$T_y(3)$</th>
<th>$C_{min}$</th>
<th>$t_{C_{min}}$</th>
<th>$V_{max}$</th>
<th>$t_{V_{max}}$</th>
<th>$V_{max,2}$</th>
<th>$t_{V_{max,2}}$</th>
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<td>ref. [11], case I</td>
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<td>1.9041</td>
<td>0.2417</td>
<td>0.9213</td>
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<tr>
<td>present study, case I</td>
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<td>0.9025</td>
<td>1.898</td>
<td>0.2421</td>
<td></td>
<td></td>
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</tbody>
</table>

4 Numerical results

4.1 Free surface flow with surface tension

The numerical results are shown for the case of a rising bubble considered in [11], where the following values were used $\rho^A = 1000 \text{kg m}^{-3}$, $\rho^B = 100 \text{kg m}^{-3}$, $\mu_A = 10 \text{Pa s}$, $\mu_B = 1 \text{Pa s}$, $f = (0, -0.98) \text{m s}^{-2}$ and $\gamma = 24.5 \text{N m}$. The height of the rectangular computational domain is $H = 2 \text{m}$ and width is $W = 1 \text{m}$. The fluid B is originally located in the circle of the diameter $0.5 \text{m}$, whose center is displaced by $0.5 \text{m}$ up from the bottom of the domain. The boundary $\Gamma_W$ contains the bottom and top of the domain, whereas $\Gamma_S$ includes the rest of the boundary (i.e. $\Gamma_I = \Gamma_D = \emptyset$).

Due to the gravity force, the fluid B with the lower density starts to rise, which also leads to a shape deformation, see Fig. 2. The computations were performed on triangular meshes with the equidistant partition. The spatial steps $h = 1/20, 1/40$ or $1/80$ were used. The step $h = 1/40$ was the coarsest mesh used in [11]. The time step used in the computation was $\Delta t = 0.002$. The motion of the domain $\Omega^B(t)$ with the area $A(t)$ was tracked in terms of the $y$–coordinate of the center of mass $T_y(t) = \int_{\Omega^B(t)} x_2 \, dx/A(t)$, the circularity defined by $C(t) = 2\pi A(t)/\int_{\partial\Omega^B} 1 \, dS$ and the rise velocity $V = \int_{\Omega^B(t)} u_2 \, dx/A(t)$. In order to verify the presented numerical method the values of $T_y$, $C$ and $V$ were computed at every time instant for both the test cases. The graphs of $T_y$, $C$ and $V$ in dependence on time shown in Fig. 1 agrees well with the results in [11].

4.2 Free surface flow with contact angles

For the second test case the two-dimensional flow of molten glass (fluid A) surrounded by a gas (air) with density $\rho_A = 1.2 \text{kg m}^{-3}$ and with its viscosity taken artificially as $\mu_A \approx 1 \text{N s}$ (fluid B). This choice of viscosity was used particularly for the purpose of numerical simulation, also the dynamic effects of fluid A flow on fluid A is almost negligible. The molten glass parameters were taken as $\rho_B = 2415.6 \text{kg m}^{-3}$, glass viscosity $\mu = 35.703 \text{N s}$ and the considered surface tension coefficient was chosen as $0.35 \text{N/m}$.

Several tests were performed. First, the numerical test with zero gravity force was considered, where due to the surface tension forces the original square shape of glass material was deformed to the equilibrium of circular shape. Second, still with zero gravity the original drop of molten glass at the boundary was deformed to an equilibrium position influenced just by prescription of different value of the static contact angles $\beta = 30, 90$ and $150$ degrees.
Figure 2: The numerical results in terms of bubble shape (left), flow velocity magnitude (middle) and pressure (right).

Figure 3: The computed steady solution for the bubble at wall in the case of zero gravity forces influenced by the prescribed static contact angle $\beta = 30$ (left), $\beta = 90$ (middle) and $\beta = 150$ degrees.
5 Conclusion

In this paper the numerical method for approximation of flow of two immiscible fluid was described. The finite element method was used based on the variational formulation of the motion equation, including also the variational formulation of surface tension terms, which allows a natural inclusion of physical phenomena known as the static contact angle. The problem was time discretized and spatially approximated by the finite element method. The XFEM was applied in order to overcome the spurious currents nearby the surface. The motion of the free surface was treated with the aid of the level set method. The presented numerical method was applied on a benchmark problem, which also includes the static contact angle treatment.

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