Two-phase flows using the XFEM: Modeling of transport phenomena on fluid interfaces

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1 Introduction

The modeling of transport phenomena on arbitrary and even moving interfaces is a topic of increasing interest in the scientific community. It is directly related to the solution of PDEs on hypersurfaces (manifolds). The field of applications for such kind of problems is widespread and can be found in fluid mechanics [2], computer graphics [3], material science [4] and biology [5]. We are considering the transport of insoluble surfactants on two-fluid interfaces in this paper.

![Diagram of Flow field, Advection/deformation of the interface, Variable surface tension, Surfactant transport on the interface](image)

Figure 1: The interaction of the different fields involved.

Figure 1 depicts the considered situation schematically. The flow field and interface representation are modeled in a coupled manner. Both influence the transport of the surfactants on the interface. Surfactants give rise to gradients in the surface tension. This leads to tangential forces along the interface and thereby couples the surfactant transport with the flow field. Though, in this work, we will not consider an influence of the surfactants on the flow field.

An important prerequisite for the accurate modeling of such interface transport phenomena is an accurate description of the flow field and the interface movement. Hence, we apply the extended finite element method (XFEM) [1] in order to account for the discontinuous nature of the field variables in two-phase flows. Thereby, we obtain an accurate implicit interface description based on the level-set method. The interface transport is modeled with an implicit approach, too.
2 Modeling of two-phase flows

The fluid velocity $u$ and pressure $p$ in both phases $j = 1, 2$ are governed by the instationary, incompressible and isothermal Navier-Stokes equations:

$$\rho_j \left( \frac{\partial u}{\partial t} + u \cdot \nabla u - f \right) - \nabla \cdot \sigma = 0 \quad \text{in} \quad \Omega_j \times [0,T],$$

$$\nabla \cdot u = 0 \quad \text{in} \quad \Omega_j \times [0,T].$$

Here, $\rho_j$ and $f$ are the density of the respective fluid phase and the external body forces. The stress tensor is defined by $\sigma(u, p) = -pI + \mu_j \left[ \nabla u + (\nabla u)^T \right]$, with $\mu_j$ being the dynamic viscosity of the respective fluid phase.

The interface $\Gamma_d$ is implicitly described using the level-set method. We define the scalar level-set field $\phi$ as a signed-distance function, i.e. the level-set value at an arbitrary point is the shortest distance to the interface. In order to account for the interface motion the level-set transport equation is solved:

$$\frac{\partial \phi}{\partial t} + u(x,t) \cdot \nabla \phi = 0 \quad \text{in} \quad \Omega \times [0,T].$$

Due to the density and viscosity differences between the phases, a kink is present in the velocity and pressure field across the interface. Additionally considering surface tension effects even leads to a jump in the pressure. As a consequence of the implicit interface description, these discontinuities across the interface occur inside elements. The XFEM offers the possibility to appropriately account for this situation by locally enriching the pressure approximation space:

$$p^h(x) = \sum_{i \in I} N_i(x) p_i + \sum_{i \in I^*} N_i(x) \cdot \left[ \psi(x,t) - \psi(x_i,t) \right] a_i.$$

$p^h(x)$ is the approximated pressure field, $N_i(x)$ is the standard finite element function for node $i$, $p_i$ is the unknown of the standard finite element part at node $i$, $I$ is the set of all nodes in the domain, $\psi(x,t)$ is the global enrichment function, $a_i$ is the unknown of the enrichment at node $i$ and $I^*$ is the nodal subset of the enrichment. We are using the so-called sign-enrichment:

$$\psi(x,t) = \text{sign}(\phi(x,t)) = \begin{cases} -1 : \phi(x) < 0, \\ 0 : \phi(x) = 0, \\ 1 : \phi(x) > 0. \end{cases}$$

3 Scalar transport on the interface

The mathematical description of transport processes is rather simple. However, solving the resulting PDEs on arbitrary, moving manifolds is not straightforward. There exist explicit and implicit approaches, see e.g. [6,9]. Using an explicit surface mesh for the discretization requires a generalization of the differential operators in the differential equation in order to account for the arbitrary hypersurface. The calculation of normal vectors of the interface or the treatment of topological changes is difficult in this case. Implicit approaches typically extend the scalar off the interface to the whole domain. This obviously increases the dimension of the problem, but the transport equation can then be solved in the whole, fixed computational domain.

We adopt an implicit approach by Adalsteinsson and Sethian [6] to model scalar advection and diffusion on implicit interfaces. Assume, the scalar quantity to be transported, $G$, is given in the whole domain $\Omega$. The transport of $G$ in $\Omega$ is defined as:

$$\frac{\partial G}{\partial t} = -u \cdot \nabla G - \nabla \cdot \left[ \sum_{i \in I} N_i(x) \sigma_i \left( \nabla \phi \right) - \kappa (\nabla G \cdot n) \right],$$
Due to the signed-distance property of the level-set field, the normal vector components can be computed directly as the normalized gradient of $\phi$. The first term on the right hand side in (6) is an advection term, the second term accounts for the change in the hypersurface shape and the last term provides diffusion.

### 3.1 Extension of the scalar quantities off the interface

The approach in the previous section is based on the assumption that the scalar $G$ is known throughout the whole domain $\Omega$. From the physical point of view $G$ is, however, only available on the interface $\Gamma_d$. In order to extend this quantity off the interface to $\Omega$ we use a technique first applied by Chen et al. [8]. The original motivation was the construction of global velocity fields for problems where only interface velocities are defined. We apply the slightly modified equation given in Chessa et al. [7]:

\[
\text{sign}(\phi) \nabla G \cdot \nabla \phi = 0 \quad \text{in } \Omega,
\]

\[
G = G_\Gamma \quad \text{on } \Gamma_d. \tag{8}
\]

The solution of Eq. (7) corresponds to an extension of $G_\Gamma$ off the interface orthogonal to the level-set field $\phi$ (cf. Fig. 2). The interface $\Gamma_d$ hereby serves as an inflow boundary. That is, if we maintain a smooth level-set field this also leads to a smooth extended scalar field.

![Figure 2: Extending $G$ off the interface orthogonal to $\phi$ [7].](image)

![Figure 3: Applying the boundary condition for the extension off $G_\Gamma$.](image)

It needs to be discussed how we apply the boundary condition (8) on an implicitly given interface. We adopt a simple approach which turned out to be sufficiently accurate:

1. Find the intersections $x_{i}^{\text{int}}$ of $\Gamma_d$ with the element edges.

2. For each cut element node $i \in I^*$ find $x^* = \min_j \|x_i - x_{j}^{\text{int}}\|$.

3. Prescribe $G_i = G_\Gamma(x^*)$ (cf. Fig. 3).

### 4 Numerical Results

We consider the surfactant transport on a rising n-butanol droplet in water. The initial spherical droplet has a radius $r = 0.0015 \text{ m}$ and physical properties $\rho_1 = 845.422 \text{ kg/m}^3$, $\mu_1 = 0.003281 \text{ kg/m/s}$ and surface...
tension coefficient $\gamma = 0.00163 \text{kg/s}^2$. The surrounding phase is defined by $\rho_2 = 986.506 \text{kg/m}^3$ and $\mu_2 = 0.001388 \text{kg/m/s}$. We choose a uniform initial surfactant distribution on the interface $G_\Gamma = 0.5$ and neglect diffusion on the interface $\sigma_H = 0$. $40 \times 40 \times 80$ hexahedral elements are used to discretize the rectangular computational domain spanning $0.006 \times 0.006 \times 0.012 \text{m}$. A time span of $0.02 \text{s}$ is observed using a time step $\Delta t = 0.0005 \text{s}$.

![Figure 4: Rising droplet with surfactant concentration.](image)

(a) $t = 0.000 \text{s}$  (b) $t = 0.005 \text{s}$  (c) $t = 0.010 \text{s}$  (d) $t = 0.020 \text{s}$

Fig. 4 shows the clustering of the surfactants at the bottom of the drop as it rises.

5 Conclusion

We successfully developed a 3D two-phase flow solver that includes the simulation of transport phenomena on the interface. The XFEM framework serves as a good basis, as discontinuities across the interface are accurately accounted for. In order to keep the advantage of an implicit interface description, we employ an implicit technique for the interface transport, too. We show how the scalar quantity on the interface is extended to the whole domain. The approach given in [6] is used to govern the scalar transport of the globalized quantity. A typical application of the approach is given by means of the simulation of surfactant transport on a rising droplet.

References