

## Topology Optimization of Capillary, Two-Phase Flow Problems

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**Abstract.** This paper presents topology optimization of capillary, the typical two-phase flow with immiscible fluids, where the level set method and diffuse-interface model are combined to implement the proposed method. The two-phase flow is described by the diffuse-interface model with essential no slip condition imposed on the wall, where the singularity at the contact line is regularized by the molecular diffusion at the interface between two immiscible fluids. The level set method is utilized to express the fluid and solid phases in the flows and the wall energy at the implicit fluid-solid interface. Based on the variational procedure for the total free energy of two-phase flow, the Cahn-Hilliard equations for the diffuse-interface model are modified for the two-phase flow with implicit boundary expressed by the level set method. Then the topology optimization problem for the two-phase flow is constructed for the cost functional with general formulation. The sensitivity analysis is implemented by using the continuous adjoint method. The level set function is evolved by solving the Hamilton-Jacobian equation, and numerical test is carried out for capillary to demonstrate the robustness of the proposed topology optimization method. It is straightforward to extend this proposed method into the other two-phase flows with two immiscible fluids.

**AMS subject classifications:** 76D55, 76D45, 76T10, 65K10, 65M60

**Key words:** Capillary, two-phase flow, topology optimization, diffuse-interface model, level set method.

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## 1 Introduction

The topology optimization method for the fluid flow was pioneered by Steven et al. [1] and Borrvall et al. [2]. Topology optimization was first used to design stiffness and com-

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pliance mechanisms [3–6], and it has been extended to multiple physical problems, such as acoustic, electromagnetic, fluidic, optical and thermal problems [2, 7–12]. Several approaches, such as the evolutionary techniques [1, 13, 14], homogenization method [3, 15], density method (solid isotropic material with penalization) [7, 16–19], level set method [20–26] and phase field method [27–34], have been developed for the implementation of topology optimization. Topology optimization of fluid flows has mainly focused on the single phase flows [18, 19, 22, 26, 35–38], and the multi-component flows without surface tension [39, 40]. The two-phase flow of immiscible fluids with surface tension plays a fundamental role in many natural and industrial phenomena. Examples can be found in the studies of capillarity, low-gravity fluid flow, hydrodynamic stability, surfactant behavior, cavitation, and droplet dynamics. For the academic and engineering requirement, this paper focuses on developing the topology optimization method for the two-phase flows of immiscible fluids.

At the interface of two immiscible fluids, the cohesive forces within the fluid and adhesive forces between the fluid and its surroundings give rise to the surface tension [41]. Due to the surface tension, the complexity on dealing with moving interfaces in two phase flows are encountered from the mathematical modeling and numerical algorithmic points of view. There are many approaches to characterize moving interfaces. The two main approaches are interface tracking and interface capturing methods. In interface tracking methods (e.g. volume-of-fluid [42], front-tracking [43], and immersed boundary [44, 45]), Lagrangian particles are used to track the interfaces, and these particles are advected by the velocity field, where the difficulties on capturing the topological changes of the moving interface are encountered. In the interface capturing methods (e.g. the level set method [46–50] and diffuse interface method [51–54]), the interface is implicitly captured by a contour of a particular scalar function, and the topological changes of the interface can be flexibly treated. Therefore, the robust interface capturing methods are more popularly used in the simulation of two-phase flows, compared to the interface tracking methods.

In topology optimization of fluid flows, the solid phase is approximated using the fluid velocity penalization method, which is implemented by adding the artificial Darcy forces into the Navier-Stokes equations [2]. Based on the fluid velocity penalization method, the no-slip boundary condition is achieved at the implicit interface between the fluid and solid phases. In the simulation of two-phase flows, the stress singularity and infinite dissipation problem are encountered near the three-phase contact line of the two-phase flow, when the no-slip boundary condition is imposed on the walls of the two-phase flow directly [55, 56]. The singularity can be solved using the slip model [55] or diffuse interface method [56]. In the slip model, the slip boundary condition with the slip velocity proportional to the tangential stress is imposed on the walls. This is incompatible with the fluid velocity penalization method. On the other hand, the diffuse interface method solves the singularity and evolves the interface and three-phase contact line based on the molecular diffusion driven by chemical potential, with the no slip condition imposed on the wall. Therefore, the diffuse interface method is the reasonable choice to