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On the streamfunction–vorticity formulation in sliding bi-period frames: Application to bulk behavior for polymer blends

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Abstract

The Lees–Edwards description of bi-periodic boundary conditions has been extended to the streamfunction and streamfunction–vorticity formulation in sliding bi-periodic frames. The required compatibility conditions are formulated and uniqueness of the solution is shown. The model has been implemented in a spectral element method context to describe bulk shear behavior far away from walls, where no simple periodic boundary conditions can be used. In the numerical model a Lagrangian multiplier is introduced to couple the shearing boundaries. The proposed method has been validated for a mathematical test problem; convergence is shown and the influence of the order of approximation of the Lagrangian multiplier is studied. Finally, results are presented for drop coalescence across the boundaries of the bi-periodic frame.

Keywords: Lees–Edwards boundary conditions; Streamfunction–vorticity formulation; Lagrangian multiplier; Polymer blends

1. Introduction

Blending or mixing of immiscible polymers offers an attractive and efficient route to produce 'new' materials with tailor made properties. The mechanical properties of these multi-phase polymer blends are intimately connected with the morphology imparted during processing. Hence, understanding the connection between applied flow and morphology development is vital to optimize the processing and therefore the

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resulting properties of blends. In the literature a large number of comprehensive experimental and theoretical studies of the morphology development in simple (shear) flow fields are reported, and some of this work is summarized in the review by Tucker and Moldenaers [1]. Although considerable fundamental understanding of morphology changes during (shear) flow has been obtained already, the prediction of the (transient) rheology coupled with the micro structure development still remains a challenge. One of the main difficulties, which is addressed in the current paper, is the correct description of bulk shear behavior far away from the shearing walls.

In 1972, Lees and Edwards [2] proposed a bi-periodic domain concept for molecular dynamics simulations by describing sliding boundary conditions for simple shear flow, which is nowadays referred to as Lees–Edwards boundary conditions. Recently, this scheme has been used with the Lattice Boltzmann method to solve particle suspension [3] and phase separation problems [4,5]. It has also been applied to concentrated emulsion problems by a Lagrangian–Eulerian method with a re-meshing technique using Voronoi tessellation [6]. Hwang et al. [7] extended the sliding bi-periodic frame concept of Lees and Edwards for discrete particles to continuous fields and combined it with the velocity pressure formulation of the fictitious-domain/finite element method.

In this study the sliding-periodic frame is used to describe drop deformation, breakup and coalescence in a shear flow. Essentially, after formulating the corresponding flow equations for a blend of two Newtonian fluids in the absence of inertia, this reduces to the description of the streamfunction–vorticity formulation for Lees–Edwards boundary conditions which is the main objective of this paper. In general for the streamfunction–vorticity formulation with Dirichlet-type of boundary conditions complicated integral type boundary conditions need to be specified in order to obtain an equivalent formulation [8].

The manuscript is organized as follows: first a description is given of the sliding-periodic frame concept and the governing equations in both a streamfunction and a streamfunction–vorticity formulation are derived. In Section 4, the weak formulation of the latter is described and equivalence of the variational problem with the original strong form is shown. Details of the implementation are given where a Lagrangian multiplier is used to couple the shearing boundaries. In Section 5 the model is validated using a mathematical test example and *hp*-convergence is shown. Finally, the streamfunction–vorticity formulation is combined with the Cahn–Hilliard theory and the process of coalescence of drops across bi-period frames is studied.

2. Sliding frames

In order to describe bulk shear behavior far away from walls, the sliding frame concept of Lees and Edwards [2] can be used. This concept is illustrated in Fig. 1. If we have a steady shear flow characterized

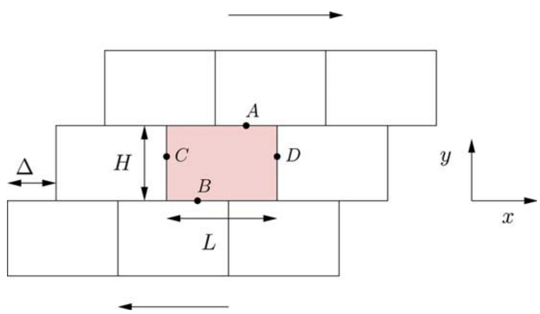

Fig. 1. Sliding frame concept of Lees–Edwards.