

LATTICE BOLTZMANN METHOD FOR MICROFLOW ANALYSIS IN LIQUID COMPOSITE MOLDING

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SUMMARY: Resin flow inside a fiber tow made of aligned fibers is an important phenomenon which occurs during the impregnation stage of Liquid Composite Molding processes. This has been previously studied using analytical and experimental methods, but there is a need to understand the capillary flow advancement at the fiber level within a fiber tow especially when it interrelates with the opposing effect due to entrapped air. This paper adopts the Lattice Boltzmann Method (LBM) to simulate the two-phase flow of impregnating resin and voids through a model geometry, which represents the fiber architecture within a fiber tow. The salient features of the LBM approach are introduced and the technique to model the capillary impregnation of resin across a fiber tow and the displacement of micro-voids is described. The potential of this technique is outlined, as it allows one to evaluate the influence of wetting characteristics of the resin on the dynamics of air entrapment and the saturation of the fiber tows. Such numerical study contributes to better understanding of the dynamics of capillary effects at the micro-scale level within a fiber tow and should prove useful to manufacture void free composites.

KEYWORDS: Capillary flow, two-phase flow, micro-scale flow, Lattice Boltzmann Method, numerical simulation, liquid composite molding.

INTRODUCTION

In Liquid Composite Molding (LCM), a composite part is manufactured by impregnating a network of reinforcements with a liquid polymer resin (filling stage). The composite part is demolded after the resin cross-links the polymer chains and the part becomes solid (curing stage). Usually, the reinforcements are bundles (tows) containing thousands of aligned fibers of micron-size diameters. These tows may be stitched, woven or braided, creating a very complex network of channels and gaps that the resin should completely fill. The structural properties of the final composite part are critically dependent on the quality of the filling stage, which should ensure that all the gaps are filled with resin. Any voids that would remain after the part solidifies, may

they be at the mold scale (dry spots or macro-voids) or of the order of the fiber scale between or within fiber tows (micro-voids) which will adversely influence the properties of the composite part. It is therefore very important to understand the factors which influence void occurrence and development during the filling stage of LCM processes, so that the manufacturing process can be designed to minimize or eliminate void content. Micro-voids in particular pose a challenge, as they are not visually detectable in the composite part, requiring involved non destructive techniques for quality assessment. Our numerical approach focuses on the formation of micro-voids between the fibers within a fiber bundle and the role of fiber arrangement and the wetting properties on micro void formation.

Previous work has been done on micro-void formation, both analytically [1] and experimentally [2, 3]. We use the Lattice Boltzmann Method (LBM) to describe the two phase flow at the microscale. The fundamentals of LBM are described and the particular model employed in our study, which compares well with results from literature is presented. The model of the solid/liquid/gas contact region is demonstrated with an example, as well as the potential of this numerical technique to further study micro-void generation and development is discussed.

THE LATTICE BOLTZMANN METHOD

Background

Flow through complex geometries, with no slip or no flow boundary conditions have been traditionally analyzed and solved using Computational fluid dynamics (CFD). CFD methods discretize the continuous flow domain into cells upon a spatial mesh in which the Navier-Stokes equations that describe the flow are solved. The flow of resins through porous media is suitable for, and has been studied with CFD tools, yet several limitations underline the need for an alternate approach. For example, one complicating factor is the fact that in LCM, two phases (gas and liquid) coexist and the flow is dual-phase. Furthermore, the significant difference in density between the two phases (by three orders of magnitude) poses additional challenges which cannot be addressed by CFD in an efficient manner.

A particularly promising class of CFD's are the Lattice Boltzmann methods (LBM), a novel approach which is an alternative to mesh-based methods, as they simulate an equivalent mesoscopic system on a Cartesian mesh, rather than solving the macroscopic system. LBM can solve a discrete equation (Boltzmann equation) to simulate the flow of a Newtonian fluid, rather than the Navier-Stokes equations. Unlike traditional CFD methods, which solve numerically the mass / momentum / energy conservation equations, the LBM uses fictitious particles whose interaction and movement over a discrete mesh describe the actual flow behavior. The basic principle of this technique is that the flow domain is considered a collection of particles which propagate in discrete preset directions and collide with one another along preset collision scenarios (Fig. 1).

The specific nature of LBM makes it more adaptable to address complex boundaries, boundary conditions and microscopic interactions at the contact region between fluid and solid obstacles, than conventional CFD. Additionally, the ability to model multi-phase flow featuring large density ratios makes LBM appealing to study micro-flow through porous media in LCM.

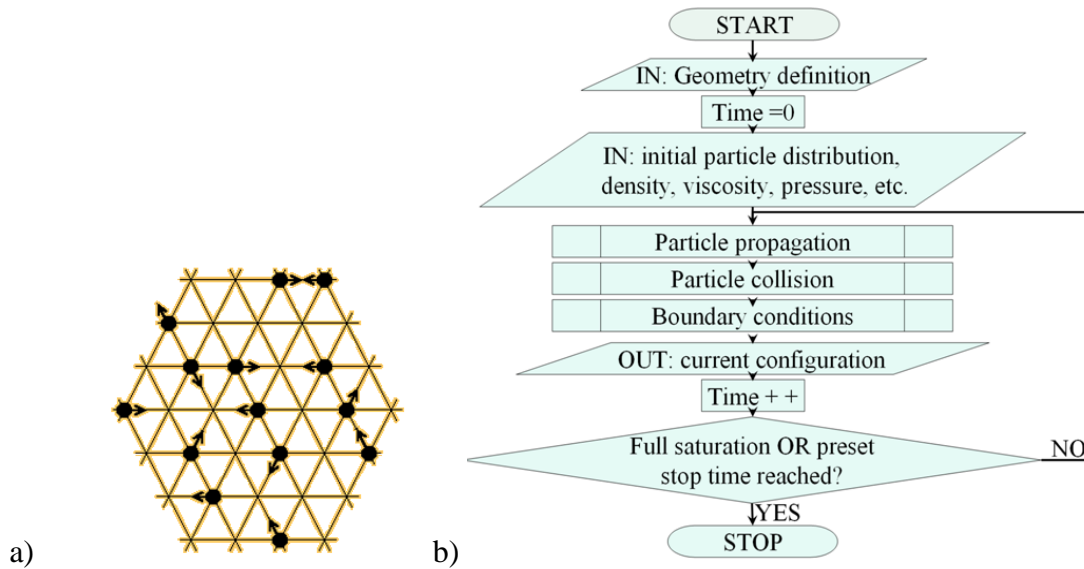


Fig. 1 a) Typical Lattice Boltzmann Method model (D2Q7), where the 2D flow domain is discretized using fictitious particles moving and mutually colliding along 7 predetermined discrete directions. b) General LBM algorithm, as a succession of particle propagations and collisions, with boundary conditions imposed at every time step.

Selection of the LBM Model

Various LBM models have been proposed and used in the past to simulate a wide range of flow scenarios. One of the most important characteristics which differentiates between various such models is the dimension of the space modeled, either in 2D (such as the example depicted in Fig. 1a) or in 3D. In our case, we are interested in modeling the flow at the microscale through a particularly complex geometry, namely an array of cylindrical fibers (Fig. 2).

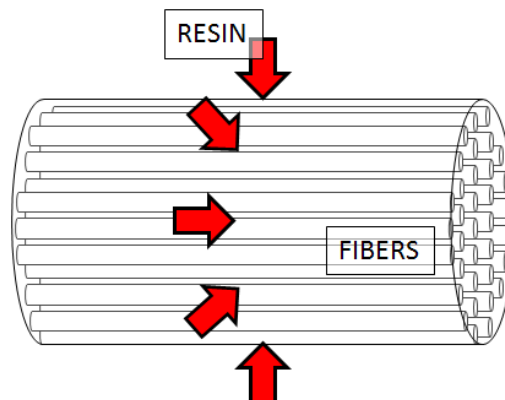


Fig. 2 The problem simulated is flow of liquid resin through an array of solid cylindrical obstacles in the presence of air.

Although adoption of simplifying assumptions (perfectly parallel alignment of fibers, ideally radial inward flow, etc) could allow the use of a 2D model, we recognized that a 3D model is

more powerful and flexible, since it could account for a larger variety of flow scenarios (e.g. non uniform fiber distribution, non parallel fiber alignments, arbitrary direction of gravitational acceleration or the local gradient of externally applied pressure, etc).

Of the available LBM models in 3D, we selected the model proposed in [4], which features 15 discrete velocities. An additional reason for the selection of this particular model is that it allows density ratios up to 1000, which is similar to the actual density ratio of resin and air.

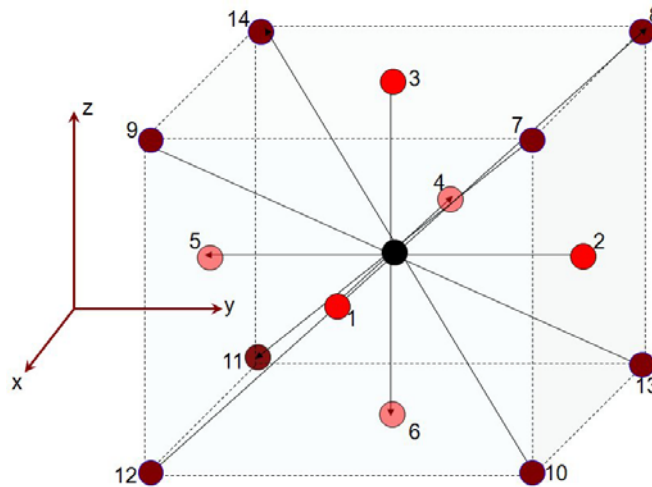


Fig. 3 Schematic of the particular Lattice Boltzmann model used in the paper (D3Q15). The flow is simulated through the collective behavior of particles, which propagate and collide along 15 predetermined directions through a discrete 3-D lattice.

LBM Code - Qualitative Validation

The approach selected was programmed in C and was built on the reference model. For qualitative validation, we simulated the upward motion of two gas bubbles, which rise exclusively due to buoyancy. The results are compared in Fig. 3, where configurations at several time steps are shown. The development of the two bubbles moving upward in tandem up to their coalescence is captured by the code, although incomplete information on the simulation parameters in the reference paper precluded us from a full quantitative comparison of our results.

- a) b) c) d) e)

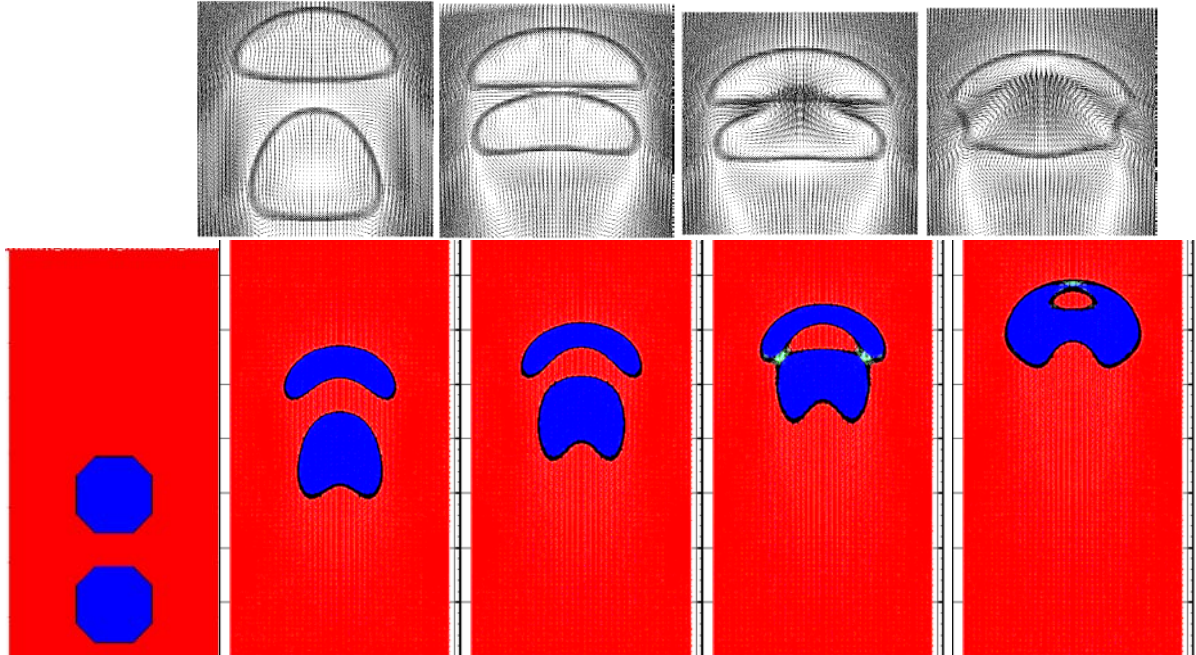


Fig. 4 Simulation of two bubbles rising due to buoyancy. Literature results (first row of images, shown as side views) and our LBM simulation (second row of images, shown as cross-sections) are compared. Results are shown at various normalized time steps:
 a) time $T = 0$; b) $T = 3.9$; c) $T = 4.6$; d) $T = 5.2$; e) $T = 6.1$.

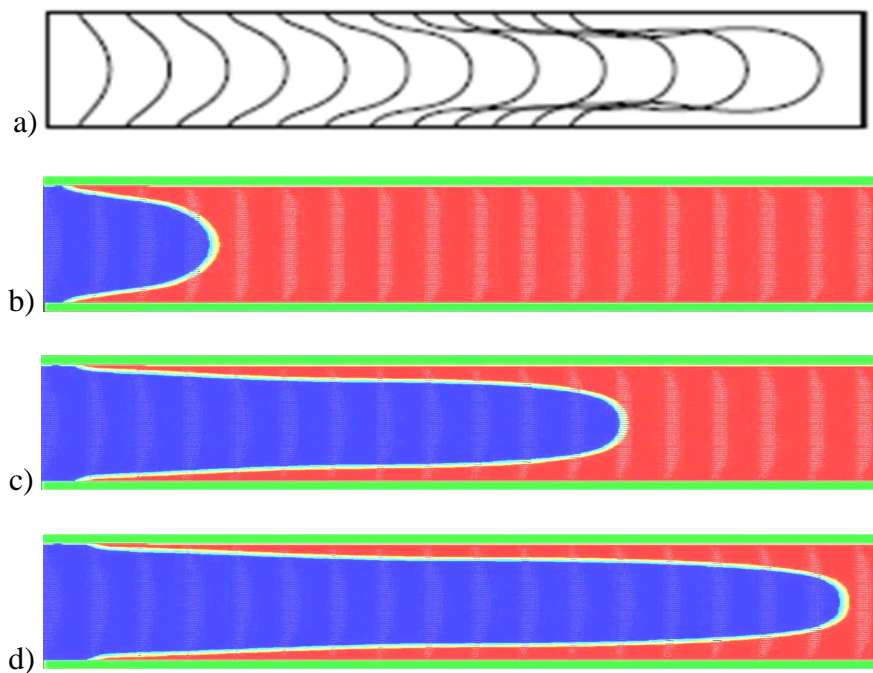


Fig. 5 Simulation of the fingering effect in two-phase flow through a channel.

The initial LBM model was further extended to simulate flow interaction with solid obstacles. This further development permits simulating the wetting mechanism between the fluid and the surface of the solid obstacle. Consequently, the code developed can simulate capillary flow at micro-scale. Qualitative comparison with literature results ([5]) is shown in Fig. 5, where flow of an incoming phase (gas, from left) displaces another phase (liquid, at right) inside a rectangular channel. The results are qualitatively similar to other results in the literature, more work being needed to ensure quantitative validation of the code.

LBM Code – Current Work

Currently, the details of the simulation of two-phase flow across an alignment of fibers is underway the flow scenario corresponds to the case of transverse impregnation of resin inside a fiber tow, driven by externally applied pressure to which capillarity contributes (Fig. 6).

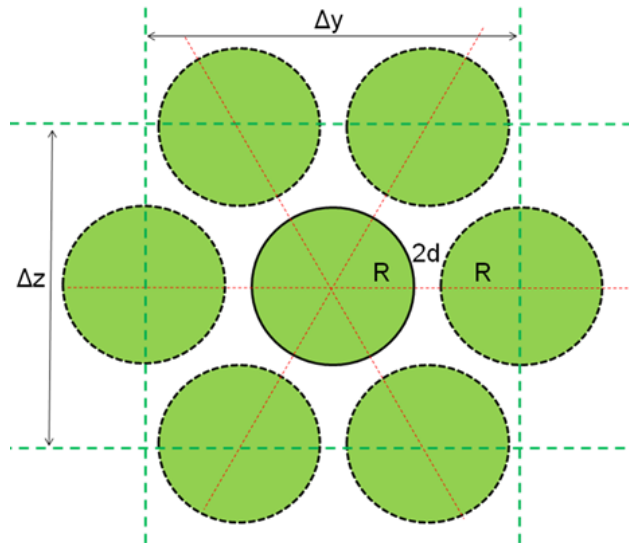


Fig. 6 Model of a cross-section through a tow made of perfectly aligned fibers. Such representative elementary cell can be used to model various scenarios of tow impregnation, depending on the boundary conditions imposed at the ends of the domain.

Variations of the impregnation scheme at the micro-scale can be tested, such as exclusive capillary impregnation, complete or gradual air entrapment, effects of various sizing agents (wetting) on the quality of fiber tow saturation.

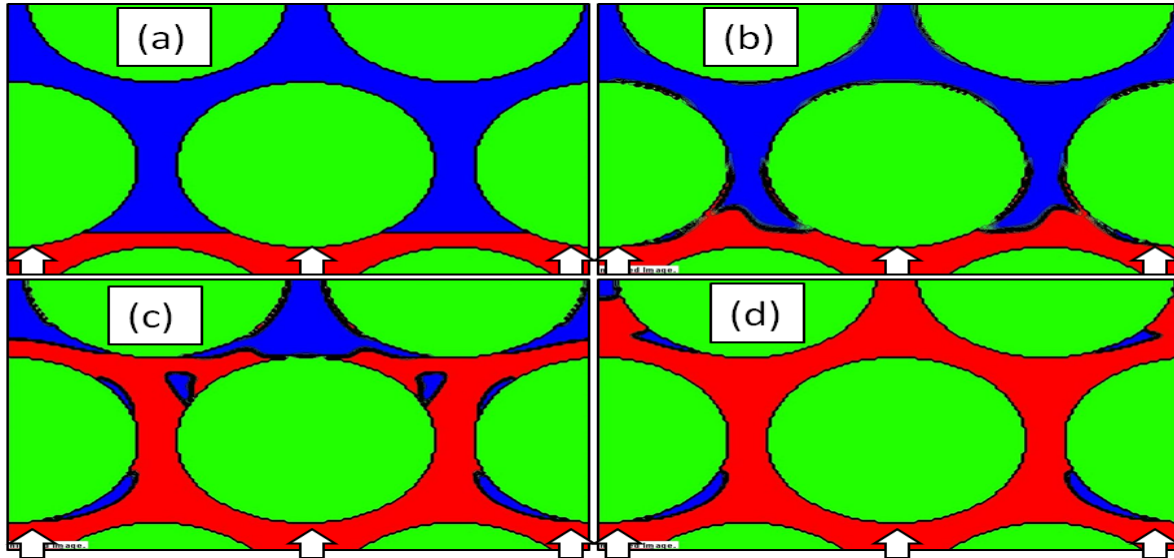


Fig. 7 Simulation of flow across an alignment of cylindrical fibers. Outside pressure pushes the liquid from the bottom of the domain upward, and capillarity assists the tow saturation. Configurations at four different time steps are shown, from a) to d).

Such a flow scenario is presented in Fig. 7, where the resin impregnates the fiber tow transversally due to applied pressure and capillarity. An escape route is provided for the air at the top of the domain, and the boundaries were left free, with the exception of the bottom edge, where incoming liquid flow was imposed. The fractions between phases and the solid regions can be used for a direct correspondence to void content and saturation factor during the process and when steady state is achieved. For example, in Fig. 7d, an approximate 1% void content is registered, in a configuration measuring 70% in fiber volume fraction. Further work is being done on ensuring that numerical instabilities are taken care of, and a direct correspondence exists between the simulation time scale and the real time scale. Also, an accurate relationship between the wetting/non wetting ability of the liquid with respect to the solid obstacle is being addressed.

LBM Code – Potential Applications

The results presented above provide a window on the possibilities LBM can offer. Impregnation of fiber tows can be modeled in more complex and realistic situations, such as when the distribution of fibers is not uniform, and the fibers are not parallel to one another. Furthermore, the code can model variations in the viscosity of the liquid during impregnation, which would simulate the gelling of a thermoset resin. Other impregnation scenarios can also be tackled, such as when the air present does not have an escape route and remains trapped inside the domain. These options will be explored soon; to assist in better understanding the mechanism of capillary impregnation of fiber tows, and the role air plays in obstructing the saturation.

CONCLUSIONS

The paper presents a novel numerical approach in the study of fiber tow saturation in LCM processes, using the Lattice Boltzmann Method. The features of the technique are briefly introduced, along with how our code was written and qualitatively validated. A typical application is presented, which illustrates the potential of the LBM code to simulate a broad range of flow scenarios in fiber tow saturation. Further work is required to eliminate the numerical instabilities, which occur at the present time, and to ensure that quantitative results such as the tow saturation time scale, and void content can be obtained.

ACKNOWLEDGMENTS

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REFERENCES

1. V. Neacsu, A. Abu Obaid, and S.G. Advani, "Spontaneous Radial Capillary Impregnation across a Bank of Aligned Micro-Cylinders - Part I: Theory and Model Development", *International Journal of Multiphase Flow*, Vol. 32, 2006, pp. 661.
2. V. Neacsu, A. Abu Obaid, and S.G. Advani, "Spontaneous Radial Capillary Impregnation across a Bank of Aligned Micro-Cylinders - Part II: Experimental Investigations", *International Journal of Multiphase Flow*, Vol. 32, 2006, pp. 677.
3. V. Neacsu, J. Leisen, H.W. Beckham, and S.G. Advani, "Use of Magnetic Resonance Imaging to Visualize Impregnation across Aligned Cylinders Due to Capillary Forces", *Experiments in Fluids*, Vol. 42, 2007, pp. 425.
4. T. Inamuro, T. Ogata, S. Tajima, and N. Konishi, "A Lattice Boltzmann Method for Incompressible Two-Phase Flows with Large Density Differences", *Journal of Computational Physics*, Vol. 198, 2004, pp. 628.
5. Q. Kang, D. Zhang, and S. Chen, "Immiscible Displacement in a Channel: Simulations of Fingering in Two Dimensions", *Water Resources*, Vol. 27, 2004, pp. 13–22.