MSc graduation project

Lattice Boltzmann Modeling of Anisotropic Homogeneous Crystal Growth with Applications to Sugar Alcohols

Introduction

Phase Change Materials (PCMs) have long been proposed as one important category of heat storage media. Recent advancement in PCM development ascribes to the discovery of a promising class of materials – Molecular Alloy based Sugar Alcohols (MASAs), under the project framework of SAM.SSA. These materials have large melting enthalpy, moderate melting temperature and significant subcooling effects, and therefore are very promising in seasonal storage applications. However the slow kinetics in the nucleation and crystal growth process remain to be improved. This task relies on a more detailed understanding of the thermodynamics and kinetics of the crystallization process. As traditional CFD methods perform poorly on phase change phenomena, we propose a more fundamental Lattice Boltzmann approach to study the initial formation of small crystal seeds, and how defects and geometric features influence the morphology and kinetics of crystal habits. The task is in conjunction with molecular level theoretical approach and experimental works.

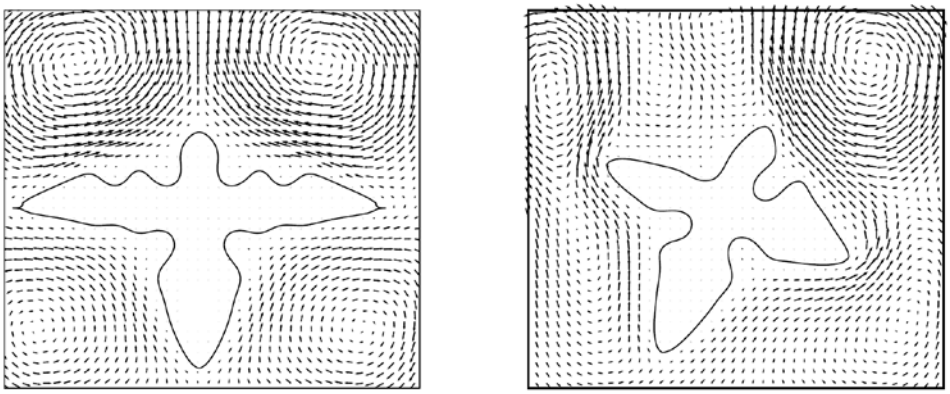

Figure 1. Velocity field around the dendrite in a Lattice Boltzmann simulation (Miller, 2001)

Methodology

The research project is based on a Lattice Boltzmann (LB) method with governing rules developed by Miller (Miller, 2001) to accommodate liquid-solid phase transition.

Tasks

- Understand LB method and the governing rules
- Write programs of 2D case
- Extend to 3D and / or perform a full investigation of 2D cases with influence of geometric features
- Comparison, validation and improvement with existing Molecular Dynamics results.
- Compose an academic paper (optional)

Requirements

- Keen to solve and contribute to global energy problems and pursue an academic career
- Good analytical and communications skills
- Basic knowledge of CFD

We Offer

- A challenging task at a dynamic and ambitious university and in an enthusiastic team
- A good entry towards state of art theoretical research and a good opportunity to **publish papers**

A consortium of 9 research institutes/companies from Germany, Spain, UK, France and Netherlands

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