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Article / Book Information

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種別(和文)	論文要旨
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（博士課程）
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論 文 要 旨

THESIS SUMMARY

系・コース： Department of, Graduate major in	機械　系 機械　コース	申請学位（専攻分野）： Academic Degree Requested	博士 Doctor of　（　工学　）
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要旨（英文 800 語程度）
Thesis Summary (approx.800 English Words)

This thesis investigates the dynamics of liquid films and bubbles in gas-liquid two-phase systems using advanced numerical simulations to overcome experimental limitations. It develops a robust computational framework employing a Weakly Compressible Scheme (WCS) with Adaptive Mesh Refinement (AMR) and GPU parallel computing to accurately capture fluid dynamics. Various numerical methods, such as interface capturing techniques and surfactant transport modeling, are integrated to study film drainage and rupture mechanisms. Special attention is given to phenomena like marginal pinching, surfactant dynamics, and the role of contaminants in bubble lifetime, offering insights applicable to environmental modeling, industrial processes, and aerosol formation.

Chapter 1 introduces the background and motivation for studying bubbles and the thin liquid films they generate. It reviews prior research on liquid film dynamics, highlighting challenges in understanding film stability and rupture due to factors like surfactant concentration, viscosity, and environmental conditions. Limitations of experimental approaches are discussed, establishing the need for numerical simulations. The research objectives focus on developing an advanced simulation framework to investigate film drainage and rupture mechanisms.

Chapter 2 presents the Weakly Compressible Scheme (WCS) utilized to simulate liquid-gas two-phase flow. It addresses challenges associated with incompressible flow simulations, particularly computational difficulties in solving the pressure Poisson equation. The WCS allows slight fluid compressibility and employs fully explicit time integration, avoiding the pressure Poisson equation while maintaining scalability and robustness. Special treatments are applied to the pressure field to mitigate acoustic oscillations. Details on discretization techniques and numerical methods, including staggered grid arrangements and calculations for advection terms and pressure gradients, are provided.

Chapter 3 overviews the interface capturing methods used in simulations. The Piecewise Linear Interface Calculation - Volume of Fluid (PLIC-VOF) method, Phase Field (PF) method, and Level Set (LS) method are discussed, each offering unique strengths in capturing interface dynamics. A coupled approach combines these methods to enhance accuracy and stability while mitigating individual limitations. The PLIC-VOF method ensures good conservation, the PF method provides a smooth interface profile, and the LS method excels at capturing sharp interfaces. The improved Height Function (HF) method is used for calculating interface curvature and minimizing spurious currents, improving the reliability of numerical simulations in complex two-phase flow scenarios.

Chapter 4 introduces the transport equations for surfactants and the Marangoni effect, emphasizing the impact of non-uniform surfactant concentration on interfacial dynamics. It describes the adsorption, desorption, and transport of surfactants within a liquid-gas system, considering the stabilizing Marangoni effect on thin liquid films. The focus is on nonionic surfactants modeled using the Langmuir model. Transport equations are solved in an Eulerian framework, allowing efficient handling of complex interfacial deformations. Detailed discretization and numerical methods ensure accurate modeling of surfactant dynamics on deformable interfaces. The Marangoni effect induced by concentration gradients is implemented using the Continuum Surface Force (CSF) model.

Chapter 5 details the use of Adaptive Mesh Refinement (AMR) and GPU parallel computing to enhance simulations. It explains the benefits of GPU computing over traditional CPU-based methods, emphasizing scalability, efficiency, and suitability for complex fluid dynamics problems. AMR dynamically adjusts grid resolution, focusing computational resources where needed—such as around rapidly changing interfaces—while maintaining coarser grids in stable regions to improve efficiency. The implementation of tree-based AMR is highlighted for its suitability on GPUs due to consistent memory access patterns. Methods for level gap interpolation ensure smooth transitions between coarse

and fine mesh regions. GPU parallel computing techniques, particularly using CUDA, exploit GPU hardware efficiently, addressing implementation challenges and ensuring accurate calculations near complex interfaces.

Chapter 6 validates the proposed numerical schemes through benchmark tests. Initial validations focus on two-dimensional tests like single vortex-induced interface deformation and surfactant transport dynamics, assessing the accuracy of interface capturing algorithms under vortex flows. The WCS is validated using 2D rising bubble simulations, demonstrating its ability to handle density and pressure variations in gas-liquid systems. Axisymmetric bubble dynamics are compared with theoretical and empirical data, confirming the robustness of the approach. Additional validations include bubble rising in viscous liquids and surfactant-laden viscous liquids, examining the thinning of the liquid film between the bubble and the free surface. Across all cases, the numerical methods show excellent agreement with reference studies, ensuring the reliability of the computational models for simulating complex multiphase fluid dynamics.

Chapter 7 investigates the dynamics of liquid films, focusing on the marginal pinching phenomenon and its effect on drainage and bubble lifetime. The chapter describes the computational domain, mesh setup, and physical properties used for simulations conducted in a 2D axisymmetric domain with fine AMR resolution. Simulations vary liquid viscosity and surfactant concentrations to explore how these factors influence the onset of marginal pinching and the drainage behavior of the liquid film. The early-stage drainage process is analyzed, emphasizing the formation of surface bubbles upon reaching the liquid surface and introducing the concept of platform thickness—a brief period where film thickness stabilizes before transitioning into late-stage drainage. Marginal pinching dynamics, including the pinching ratio and length, are explored, showing how viscosity and surfactant concentration affect the rate and extent of pinching. This process leads to the separation of the liquid film from the meniscus, affecting overall drainage. The influence of marginal pinching on late-stage drainage is examined by improving a model based on capillary pressure and viscous drag, confirming a power-law relationship for film thickness decay. The model is validated against numerical simulations, with high agreement for cases involving low surfactant concentrations and viscosities. For higher surfactant concentrations, inverse Marangoni flow driven by surface tension gradients is incorporated to explain the extended film lifetimes observed. The transverse contamination mechanism is investigated, presenting a theoretical model to predict film rupture thickness based on contaminant transport across the film. The model accurately predicts rupture thickness and drainage duration in most cases, demonstrating the importance of marginal pinching and contamination mechanisms.

Chapter 8 summarizes the key findings and contributions made through the development of advanced numerical simulations to study liquid film dynamics and bubble interfaces.