No.1

フェーズフィールドモデルに基づく 二相流界面追跡計算法

Phase-Field Method for Interface-Tracking Simulation of Two-Phase Flows

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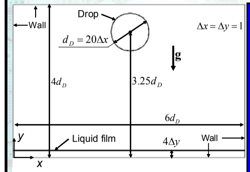
2005年6月28日(火), 東京・市ケ谷

JSAE June 19-23, 2005, Ichigaya,Tokyo,JAPAN

No.2

本講演の「フェーズフィールド法」

従来アルゴリズム・界面モデルを使用せず二相流界面捕獲追跡が可能な計算法

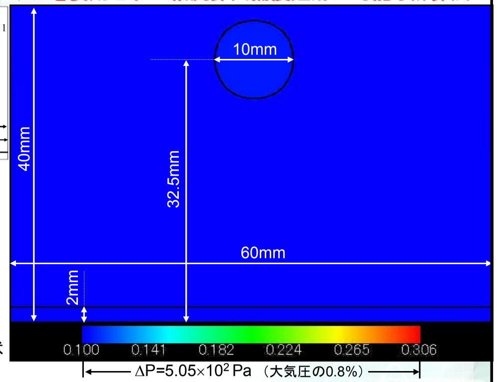


(a) 計算領域の初期・境界条件

自由落下液滴—壁面上液膜の衝突・合体数値実験（2D）

空気-水相当：ρ_L/ρ_G=801.7

μ_L/μ_G=73.76



(b) 圧力&流速分布・界面形状

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No.3

Outline

Purposes of This Study

(1) Examination of phase-field model (PFM) for tracking two-phase fluid interface

(2) Development of PFM-based computational method for interface-tracking simulation of two-phase flows

Contents

1. Basis of PFM
2. Phase-field methods (NS-PFM) combining Navier-Stokes (NS) equations with PFM for,
   (1) Isothermal fluid at a high density ratio
   (2) Thermal fluid with phase change
3. Numerical result of two-phase flows
4. Conclusions

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No.4

Phase-Field Model（PFM）

- Diffuse-Interface Model -

A useful tool for understanding complex phenomena involving self organization of mesoscopic multi-component structures in,

- Two-phase flows
  (bubbly flow, drop breakup, Rayleigh-Taylor instability, phase change）
- Solidification of binary alloys
- Polymer membrane formation（M.Doi,OCTA）

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No.5

Phase-Field Model (PFM) Based on van-der-Waals or Cahn-Hilliard Free-Energy Theory

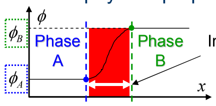
- Two-phase coexistence by a free-energy functional F :

$$F = \int \left[f(\phi) + \frac{\kappa}{2} |\nabla \phi|^2 \right] d\mathbf{x}$$

$f(\phi)$: Bulk energy (double-well for ϕ)
ϕ : Index function to describe interface
κ : Capillary coefficient

without imposing topological constraints on interface as phase boundary.

- Interface = *Volumetric transition zone* with steep & continuous variation of physical properties (density ρ, viscosity μ, etc.)



Interface thickness $l_\phi \propto \sqrt{\kappa}$

- Surface tension σ = *Excessive energy* per unit area induced by local gradient of ρ or ϕ inside interface zone

$$\sigma = \kappa \int_{-\infty}^{+\infty} \left(\frac{\partial \rho}{\partial x} \right)^2 dx$$

(for flat interface perpendicular to x axis)

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No.6

Phase-Field Model (PFM) Method for Two-Phase Flow Simulation

- PFM method does *not necessarily* require conventional,
  (1) Interfacial advection-reconstruction algorithms
  (2) CSF (Continuum Surface Force) model
- Simplified interface-tracking calculation on a fixed spatial grid
- Advantages of PFM method over others,
  Easy implementations of
  (1) multi-dimensional interface advection
  (2) heat & mass transfer across interface
- Classical NS-PFM for low density ratio ρ_L/ρ_g (due to numerical instability)
- A new NS-PFM proposed by extending a lattice Boltzmann method (LBM) for high ρ_L/ρ_g up to 1,000
- NS-PFM has lower computational cost & more flexibility than LBM.

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No.7

二相流界面追跡計算法の構成
従来法／Phase-Field Method (PFM)

巨視的現象の記述法 流れの基礎方程式	+	界面現象の記述方式 界面移流・再構成法／表面張力計算法	=	二相流数値計算手法	数値計算手法の具体例
plain Navier-Stokes (NS) Method	+	I/F-Tracking Scheme／CSF model	=	Conventional NS Method	Front-Tracking Level-Set Marker-and-Cell Volume-of-Fluid
plain LBM	+	Phase-Field Modeling (PFM)	=	Two-Phase Fluid LBM	Inamuro,T., etal. Seta,T., etal. Swift,M.R., etal.
plain-NS Method	+		=	NS-PFM	Doi,M.,etal(1997-) Jacqmin,D. (1999) Jamet,D.,etal. (2001)

＊注：支配方程式の離散化スキーム，計算アルゴリズム，座標系，等は3者とも任意選択可能

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No.8

Navier-Stokes Phase-Field Method (NS-PFM) for Incompressible Isothermal Two-Phase Flow with High Density Ratio ρ_L/ρ_G

Mass & Momentum Conservation Equations for Two-Phase Flow:

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho = 0 \qquad \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla \cdot \mathbf{P} + \nabla \cdot \left[\mu(\rho)\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right)\right] + (\rho - \rho_k)\mathbf{G}$$

Pressure tensor : $\mathbf{P} = \left(P' - \kappa_S |\nabla \rho|^2\right)\mathbf{I} + \kappa_S \nabla \rho \otimes \nabla \rho$

κ_S : Surface tension parameter

$$\sigma \equiv \kappa_S \int_{-\infty}^{+\infty} \left(\frac{\partial \rho}{\partial x}\right)^2 dx$$

* Density : $\rho(\phi) = \frac{\rho_L + \rho_G}{2} + \frac{\rho_L - \rho_G}{2} \sin\left(\frac{\phi - (\phi_L + \phi_G)/2}{\phi_L - \phi_G} \pi\right)$

* Viscosity : $\mu(\rho) = \frac{\mu_L - \mu_G}{\rho_L - \rho_G}(\rho - \rho_G) + \mu_G$

Cahn-Hilliard (CH) Equation with Advection of Fluid Interface & Volume:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = -\nabla \cdot \left[-\Gamma(\phi) \nabla \eta\right]$$

(*R.H.S.* $= 0$ *for a local equilibrium state*)

Chemical potential : $\eta = \frac{\partial \psi_\phi}{\partial \phi} - \kappa_\phi \nabla^2 \phi$

ψ_ϕ : Bulk free energy $= \phi T \ln\left[\phi / (1 - B\phi)\right] - A\phi^2$ (van-der-Waals*)

Mobility : * $\Gamma(\phi) = \Gamma \phi > 0$

κ_ϕ : Interface thickness parameter $l_\phi \propto \sqrt{\kappa_\phi}$

* Original : LBM by Inamuro,T.*etal.*, *J.Comput.Phys.*, **198**(2004), 628.

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No.9

Navier-Stokes Phase-Field Method (NS-PFM) for Thermal Two-Phase Flow with Phase Change

A Full Set of Navier-Stokes Conservation Equations for Compressible Non-ideal Fluid

ρ : Density $\mathbf{u}$: Velocity T : Temperature

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0 \qquad \frac{\partial \rho\mathbf{u}}{\partial t}+\nabla\cdot(\rho\mathbf{u}\mathbf{u})=\nabla\cdot(-\mathbf{P}+\boldsymbol{\tau})$$

$$\frac{\partial E}{\partial t}+\nabla\cdot(E\mathbf{u})=\nabla\cdot\left[(-\mathbf{P}+\boldsymbol{\tau})\cdot\mathbf{u}+k\nabla T-\kappa_S\rho(\nabla\cdot\mathbf{u})\nabla\rho\right]$$

van-der-Waals Equation of State

$$p=\frac{\rho T}{1-B\rho}-A\rho^2$$

κ_S : Parameter of σ

k : Thermal conductivity

$$E=\frac{1}{2}\rho\mathbf{u}^2+\rho(cT-A\rho)+\frac{\kappa_S}{2}|\nabla\rho|^2$$: Total energy of fluid (c : Specific heat)

$$\mathbf{P}=\left(p-\kappa_S\rho\nabla^2\rho-\frac{\kappa_S}{2}|\nabla\rho|^2\right)\mathbf{I}+\kappa_S\nabla\rho\otimes\nabla\rho$$: Pressure tensor

$$\boldsymbol{\tau}=-\frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}+\mu(\nabla\mathbf{u}+\nabla\mathbf{u}^T)$$: Viscous stress (μ : Viscosity)

Numerical solution of NS eqs.+E.O.S. :
(1) MacCormack scheme (+ explicit artificial viscosity)
(2) κ_S, c, k, μ = constant in whole flow field

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No.10

二相流界面追跡に関する従来計算法とフェーズフィールド法(PFM)との比較

	従来計算法(NS方程式)	PFM
計算法（細分類）	MAC VOF Level Set Front Tracking MPS	NS-PFM / LBM LGCA
界面厚さ	数値的（0 or ≈Δx）	物理的（>Δx, 数セル）
表面張力	Continuum Surface Force (CSF) Model（界面厚さと関連なし）	界面自由エネルギー（界面厚さと関連あり）
界面移流・再構成	MAC PLIC MARS DA TVD CIP	化学ポテンシャル勾配
離散化	Eulerian / Semi/Fully-Lagrangian / ALE — FDM FEM BEM／BFC	

PFMは新しい二相流計算アルゴリズムを提供する.

「従来法 v.s. PFM」は不十分／両者の最適な取捨選択・融合

LBM: Lattice Boltzmann Method LGCA: Lattice Gas Cellular Automaton

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No.11

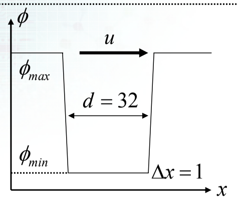
Benchmark of Transport of Interface Using Cahn-Hilliard(CH) Equations

(1) 1D Linear Transfer on a fixed spatial grid

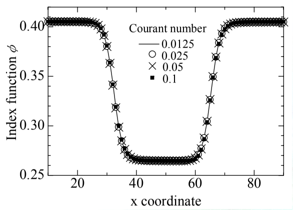
Generally, $\frac{\partial \phi}{\partial t}+\nabla\cdot[\phi\mathbf{u}+\Gamma(\phi)\mathbf{j}]=0 \quad \mathbf{j}=-\nabla\eta$

CH Equation $\Gamma(\phi)=\Gamma_0\phi$:Mobility $\Gamma_0>0$:constant

In this study, $\frac{\partial \phi}{\partial t}+\nabla\cdot[\phi\mathbf{u}+\Gamma_0\mathbf{J}]=0 \quad \mathbf{J}=-\phi\mathbf{j}=-\zeta\nabla\phi+\kappa_2\phi\nabla(\nabla^2\phi)$



Case (A) 1D square-wave propagation.



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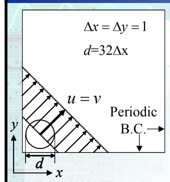
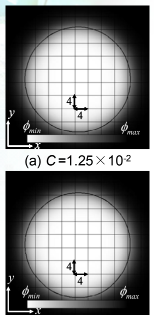
No.12

Benchmark Test on Interface Advection Using the Cahn-Hilliard (CH) Equation

(2) 2D Linear Transport



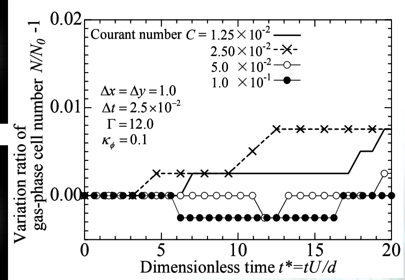
Computational domain



(a) C=1.25×10^{-2}

(b) C=2.5×10^{-2}

Interface profile at t^*=200.
(drawn as a contour line)



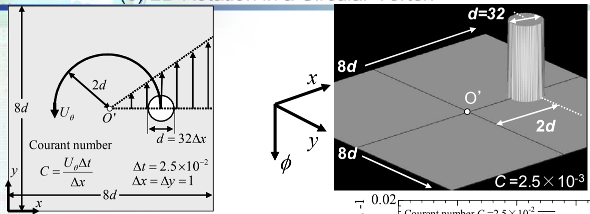
Time series of volume of circular-shaped fluid .

Parameters in CH eq.: $A=B=1$, $T=0.293$, $\kappa_\phi=0.1$

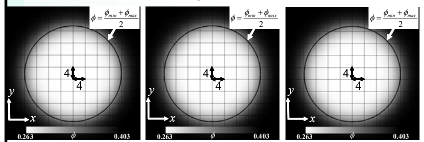
No.13

Benchmark Test of Interface Advection Using the Cahn-Hilliard (CH) Equation

(3) 2D Rotation in a Circular Vortex

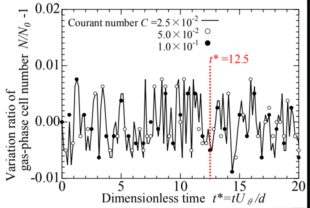


Schematics of computational domain.



C =2.5×10^{-2} C=5×10^{-2} C=10^{-1}

Interface profile drawn as a contour line of ϕ at t^*=12.5.



Volume conservation.

No.14

Cahn-Hilliard方程式を用いた界面移流問題ベンチマークのまとめ

化学ポテンシャル勾配に起因する指標関数ϕの流束の役割

(a) 高精度の体積保存性の実現

(b) 自動的な界面形状再構成の実施

・・・既存アルゴリズムなしに界面形状・厚さを一定に保持

(c) 数値拡散と数値振動の適切な抑制

・・・標準的な有限体積スキーム・時間進行法のみ使用

二相流界面追跡計算における要求への対応

(1)形状保存性 ・・・ 界面形状の正確な捕獲と輸送

(2)体積保存性 ・・・ 流体体積率の正確な輸送

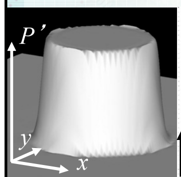
(3)流体率の連続性 ・・・勾配を考慮した界面再構成

No.15

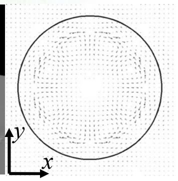
Surface Tension Force of NS-PFM

(2D Neutrally-Buoyant Bubble in Liquid)

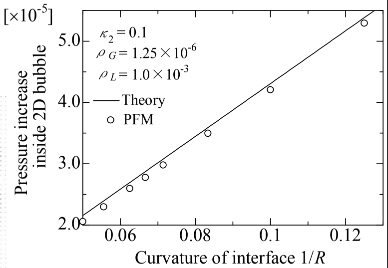
ρ_L/ρ_G =801.7
μ_L/μ_G =73.76 (for air-water system)
σ =4.31×10^{-4}



(a) Pressure



(b) Velocity

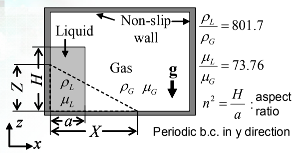


(c) Pressure increase inside bubble.

No.16

Collapse of 2D Liquid Column under Gravity

(1) Initial & Boundary Conditions



Schematic of computational domain

Table1 Parameters in liquid column simulation
(|g|=2×10^{-3}, ρ_L= 1, ρ_G= 1.25×10^{-3}, Δt = 0.0125)

Case#	Aspect ratio $n^2=H/a$	Width of column a: PFM (Δx=1)	Width of column a: air&water (m)	Surface tension σ	Viscosities: μ_G (gas)	Viscosities: μ_L (liquid)
1	2	10Δx	1.46×10^{-1}	7.11×10^{-5}	1.43×10^{-7}	1.06×10^{-5}
2		18Δx		2.30×10^{-4}	3.47×10^{-7}	2.56×10^{-5}

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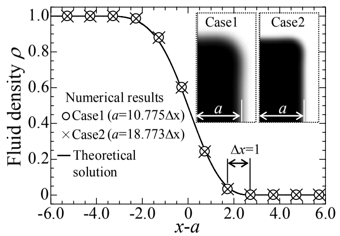
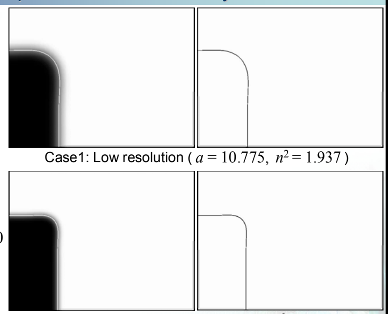
Collapse of 2D Liquid Column under Gravity

No.17

(2) Thickness Profile, Shape of Column & Velocity Field



Initial profile of fluid density ρ across liquid-column interface on a bottom wall surface



(a) Shape of column (b) Interface and velocity

Movies of collapsing liquid column

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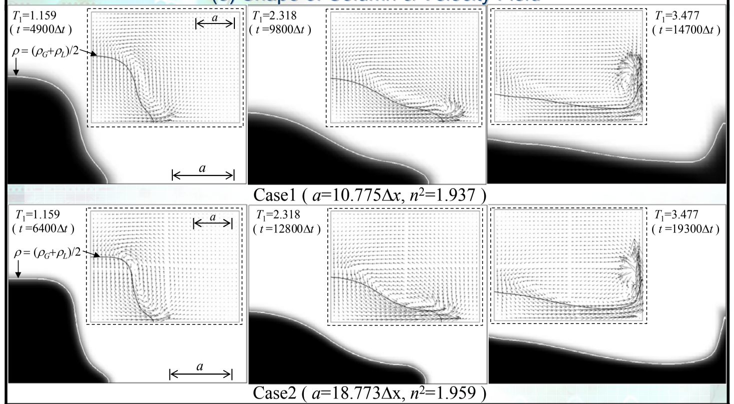
Collapse of 2D Liquid Column under Gravity

No.18

(3) Shape of Column & Velocity Field



(1) t_{aw} = 0.1s (2) t_{aw} = 0.2s (3) t_{aw} = 0.3s

* t_{aw} for a=0.146m in air-water system.

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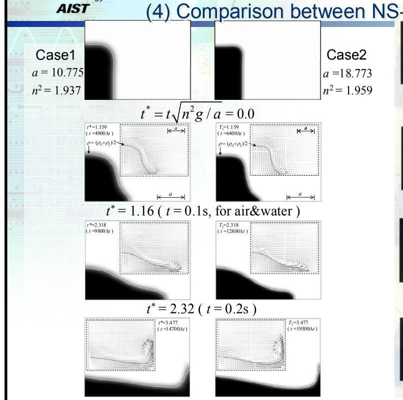
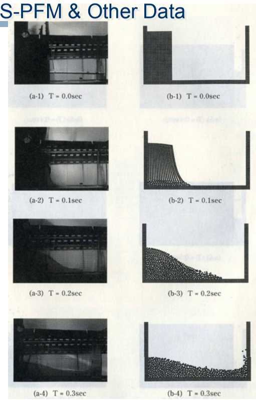
Collapse of 2D Liquid Column under Gravity

No.19

(4) Comparison between NS-PFM & Other Data



Numerical solutions by NS-PFM



* Experimental result (a=146mm, n^2=2)
* Numerical sol. by MPS method (a=18, n^2=2)

* Ref. Koshizuka&Oka, Nucl.Sci.Eng.**123**(1996),421-434.

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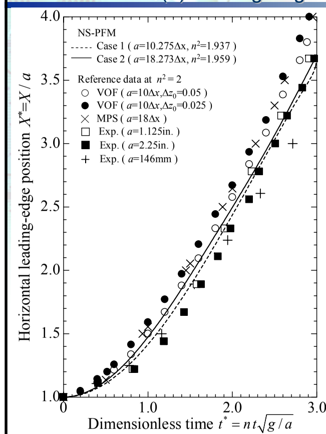
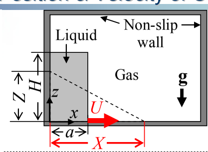
Collapse of 2D Liquid Column under Gravity

No.20

(5) Leading-Edge Position & Velocity of Column



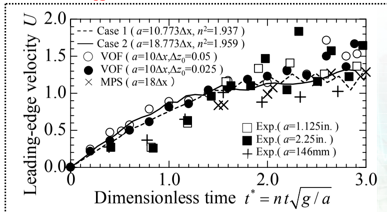
Time series of horizontal leading-edge position X



Density ratio : $\frac{\rho_L}{\rho_G} = 801.7$

Viscosity ratio : $\frac{\mu_L}{\mu_G} = 73.76$

Aspect ratio : $n^2 = \frac{H}{a} \cong 2$



Time series of horizontal velocity U of leading edge

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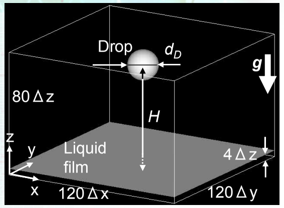
No.21

Coalescence of Free-Fall Single Drop into Stagnant Liquid Film in 3D



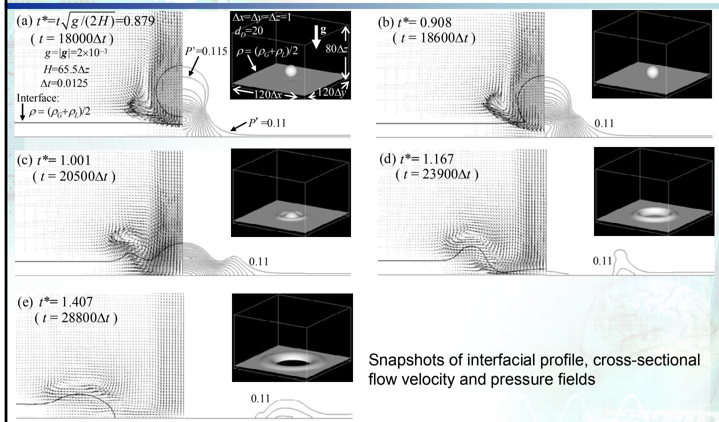
Computational domain and Interfacial profile of liquid film and free-fall drop with diameter d_D=20 and initial height H=65.5Δz

Fluid : Air-Water (1atm, room temp., d_D =10mm)
Density ratio : ρ_L/ρ_G = 801.7
Viscosity ratio : μ_L/μ_G = 73.76
Eötvös number : Eo = 13.2
Morton number : $M = 1.52\times10^{-12}$
Boundary condition : Solid walls (contact angle 90°)

ρ_L =1.0	d_D=20
ρ_G =1.25×10^{-3}	Δx=Δy=Δz=1
μ_L =1.67×10^{-3}	|g| =2.0×10^{-3}
μ_G =2.26×10^{-5}	Δt =1.25×10^{-2}
σ =6.06×10^{-2}	

No.22

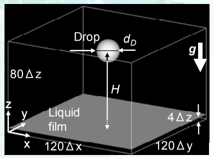
Coalescence of Free-Fall Drop & Stagnant Liquid Film in 3D

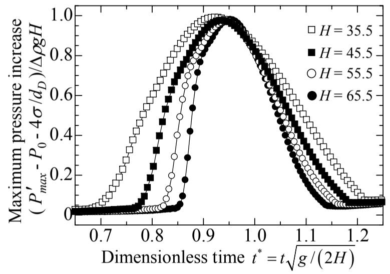


Snapshots of interfacial profile, cross-sectional flow velocity and pressure fields

No.23

Coalescence of Free-Fall Drop & Stagnant Liquid Film in 3D



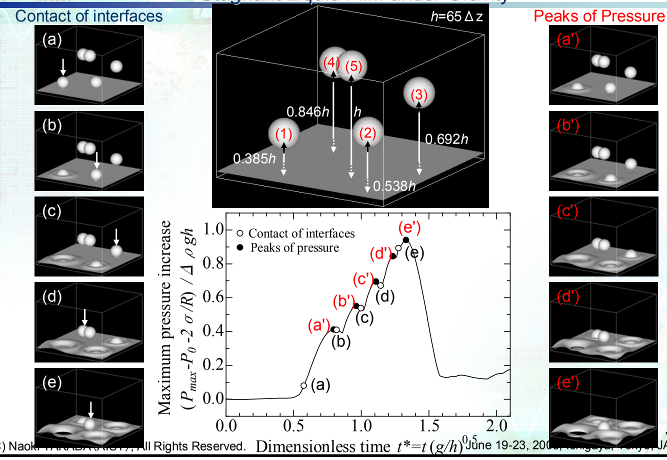


Time series of maximum pressure P'_{max} for initial height H of drop with d_D at dimensionless time t^*

No.24

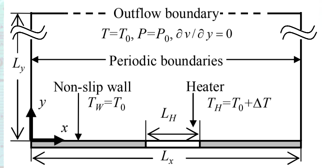
Numerical Simulation by NS-PFM

Coalescence of 3D Liquid Drops and Stagnant Liquid Film under Gravity

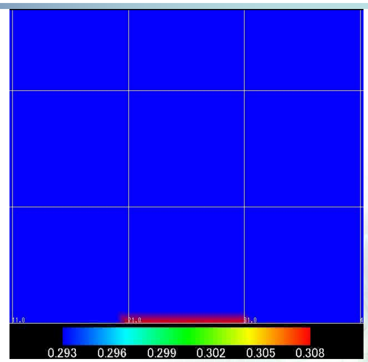


No.25

DNS of 2D Bubble Nucleation in a van-der-Waals Fluid



Computational domain



Time evolution of interface profile, velocity and temperature fields

Parameters

van-der-Waals fluid : $A=B=1$

Specific heat: $c=1$

Density : $\rho_L=0.405$

Surface tension coefficient : $\kappa_S=0.01$

Thermal conductivity : $k=0.2$

Viscosity : $\mu=0.2$

Gravity : $|\mathbf{g}|=g=0$

Temperature :

$T_0=0.293$

$T_W=T_0$

$T_H=T_0+\Delta T$

$\Delta T=0.05T_0$ ($=1.465\times10^{-2}$)

Discretization of space&time :

$\Delta x=\Delta y=1$ $\Delta t=0.2$

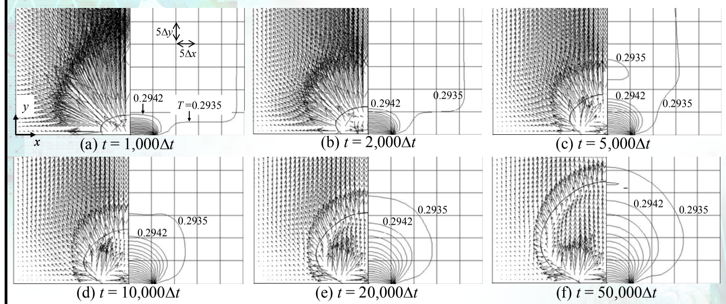
$L_x=L_y=50$

$L_H=10$

JSAE June 19-23, 2005, Ichigaya, Tokyo, JAPAN

No.26

2D Bubble Nucleation in Non-Ideal Fluid



Snapshots of interface profile, velocity and temperature fields

2D bubble nucleated on heater with width $L_H=10\Delta x$ in a van-der-Waals fluid at time t, $\Delta x=\Delta y=1$, $\Delta t=0.2$.

JSAE June 19-23, 2005, Ichigaya, Tokyo, JAPAN

No.27

Conclusions

For interface-tracking simulation of two-phase flows, we proposed two versions of phase-field method, NS-PFM, combining Navier-Stokes (NS) equations with phase-field model (PFM).

It was confirmed through numerical simulations that,

(1) The flux driven by a chemical potential gradient in the Cahn-Hilliard equation plays an important role in interface advection and reconstruction.

(2) The first version of NS-PFM gives good predictions of incompressible, isothermal two-phase flows at a high density ratio.

(3) The second version of NS-PFM successfully reproduces liquid-vapor interface motion with heat transfer in non-ideal fluid in the vicinity of critical point.

JSAE June 19-23, 2005, Ichigaya, Tokyo, JAPAN

No.28

謝　辞
（ 敬称略 ）

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神戸大学

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研究実施制度　文部科学省 科学技術振興調整費・流動促進研究課題（若手育成型）

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JSAE June 19-23, 2005, Ichigaya, Tokyo, JAPAN

No.29

高効率・高密度比二相流界面追跡計算法（ナヴィエ・ストークス-フェーズフィールド法:NS-PFM）の基盤開発と適用

格子ボルツマン法（LBM）の発展型計算法 ＝ 計算流体力学（CFD）＋ 非平衡系熱力学

マルチスケール＆ マルチフィジックス

― 利点 ―

（1）従来計算法より**簡素＆高効率**　（2）LBMより**柔軟な解析適応能力**

― 得意分野 ＝ 環境流体科学 ―

（1）液滴・気泡クラスター挙動・・・**汚濁水質のマイクロバブル改善技術**

（2）多孔体内二相流（毛管現象）・・・**地下水 / Diesel粒子回収Filter / 化学分析チップ（μ-TAS）**

（3）その他：相変化・溶解（界面を通過する熱物質輸送計算）

― 新規性 ―

計算技術面：

（1）NS-PFM適用の気液二相流計算・・・**国内初**

（2）高密度比対応可能なNS-PFM・・・**国内外初**

学術面：

界面追跡での自由エネルギー理論の重要性を指摘・・・**国内初**

JSAE

June 19-23, 2005, Ichigaya, Tokyo, JAPAN

No.30

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JSAE

June 19-23, 2005, Ichigaya, Tokyo, JAPAN

No.31

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Phase-Field Method for Interface-Tracking Simulation of Two-Phase Flows
URL: http://staff.aist.go.jp/naoki-takada/phase_field_cfd.htm

Lattice Boltzmann Method (LBM)
URL: http://staff.aist.go.jp/naoki-takada/lbm_study.htm

JSAE

June 19-23, 2005, Ichigaya, Tokyo, JAPAN

No.32

Information

DSFD2005（August 22-26, Kyoto Univ.）
URL: http://fd.kuaero.kyoto-u.ac.jp/DSFD2005/index.html

ICMMES2005 (July 26-29, Hong Kong Polytechnic Univ.)
URL: http://www.icmmes.org/

格子ボルツマン法の基礎と応用に関する研究分科会
（LBM研究会, A-TS05-19, JSME 流体工学部門）
URL: http://www.jsme.or.jp/

JSME 18th **計算力学講演会・OS「格子ガス・ボルツマン法」**
（2005年11月19-21日,筑波大学, 講演募集中）
URL: http://www.jsme.or.jp/cmd/cmc2005/

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