Institute of Process and Particle Engineering
Graz University of Technology

Comparative Study of the Accuracy of a DNS Solver for Fluid-Gas-Particle Flow Simulation

Mingqiu Wu,[a] Johannes Khinast,[a,b] Stefan Radl[a]

Funding for this research was provided by the Austrian Science Foundation (FWF) through Projects P23617

[a]Graz University of Technology,
Institute of Process und Particle Engineering, Graz, Austria
[b]Research Center Pharmaceutical Engineering GmbH, Graz, Austria

Introduction

The flow of liquid films is observed in many industries and in nature, e.g., coating applications in the pharmaceutical industry, or the spreading of liquid on granules in food processing. In such a flow process, the fluid is driven by gravity and the inertia, and effects due to a finite wetting speed are often small and are hence neglected [1]. While these flows have been extensively investigated by means of laboratory experiments and theory [2], theoretical concepts cannot be easily extended to investigate flows involving complex topology.

We used our newly developed DNS solver to simulate the gravity driven thin film flow on a spherical substrate, and compare our simulation results with the theoretical predictions of Takagi [1].

Simulation Method

The governing equation for the multi-fluid and fluid-particle system are given as follows:

- **Naver-Stokes equation**

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = -\frac{1}{\rho}\nabla^2\vec{u} + \vec{f}_s + \vec{f}_g + \vec{g} \quad (1)$$

- **Continuity Equation**

$$\nabla\cdot\vec{u} = 0 \quad (2)$$

- **Colour Function**

$$\frac{\partial \alpha}{\partial t} + (\vec{u}\cdot\nabla)\alpha = 0 \quad (3)$$

The VOF color function $\alpha(0 \le \alpha \le 1)$ is an indicator to distinguish between the gas and the liquid phase. The local density and viscosity of the fluid are calculated as follows:

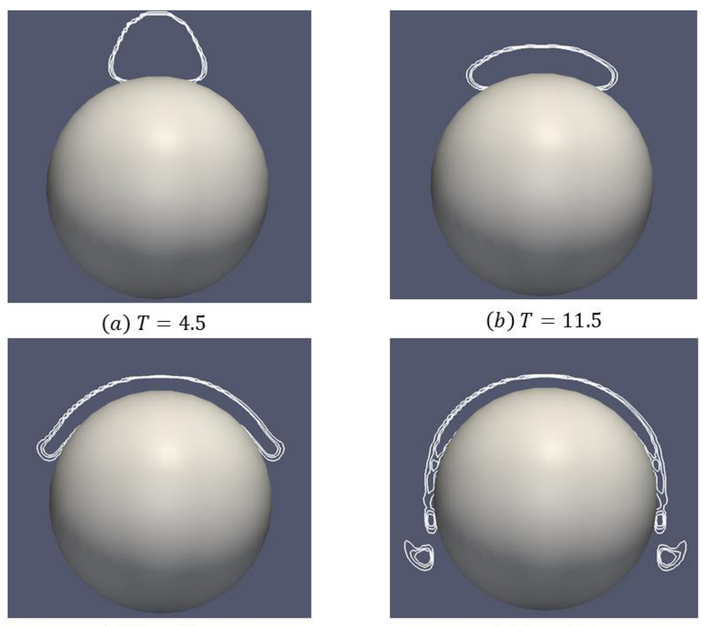
$$\rho = \alpha\rho_l + (1-\alpha)\rho_g \quad (4)$$

$$\mu = \alpha\mu_l + (1-\alpha)\mu_g \quad (5)$$

Our DNS approach is based on the immersed boundary method to model fluid-particle interaction while the volume of fluid approach for modeling a deformable fluid-fluid interaction forces.

Results

Our work connects to the theoretical and experimental study of Takagi et al. [1], which used lubrication theory to describe the flow of thin films on spherical substrates.



$(a)\ T = 4.5$ $(b)\ T = 11.5$ $(c)\ T = 45$ $(d)\ T = 86$

Fig. 1: Snapshots from a simulation of liquid spreading on a sphere. (a) $T = 4.5$ after telease, the droplet starts to spread on the sphere. (b) $T = 11.5$, the film continues to spread on the surface. (c) $T = 45$, wave patterns begin to develop at the leading edge of the film. (d) $T = 86$, droplets form and detach from the film($Bo_V = 100, Re = 1, \frac{v_l}{v_g} = 100, \frac{\rho_l}{\rho_g} = 10, \frac{V}{R^3} = 0.113$).

Software
Computations have been performed using OpenFOAM® (http://www.openfoam.org), as well as a modified version of LIGGGHTS and CFDEM (www.cfdem.com).

Rel. Domain Size	Rel. Droplet Radii	Grid Size Δx	Loss of Mass (%)
$4 \times 4 \times 4\ R$	$0.3\ R$	$d_p / 10$	9.36
		$d_p / 15$	8.81
		$d_p / 20$	8.41
		$d_p / 25$	5.41

Table. 1: Mass loss as a function of mesh resolution ($d_p = 2R$ is the sphere diameter)

We present results of a test case in which a small droplet is released on the top of a spherical particle (Fig. 1). The droplet starts to spread on the surface of the sphere, and gravitational forces lead to the detachment of droplets from the film. We check the mass conservation problem of the liquid phase value α by decreasing the mesh size of the computational domain gradually. We observe that the loss of liquid phase α value decrease from 9.36% to 5.41% when the mesh size reduced from one-tenth to one twenty-fifth of the particle diameter (see table 1). We then choose the set of parameters of the most accurate case (i.2.,case 4 in table 1) to setup the simulation. We compare the simulation results ("IBSolver") with the theoretical prediction ("Theory") of Takagi [1] (see Fig. 2).

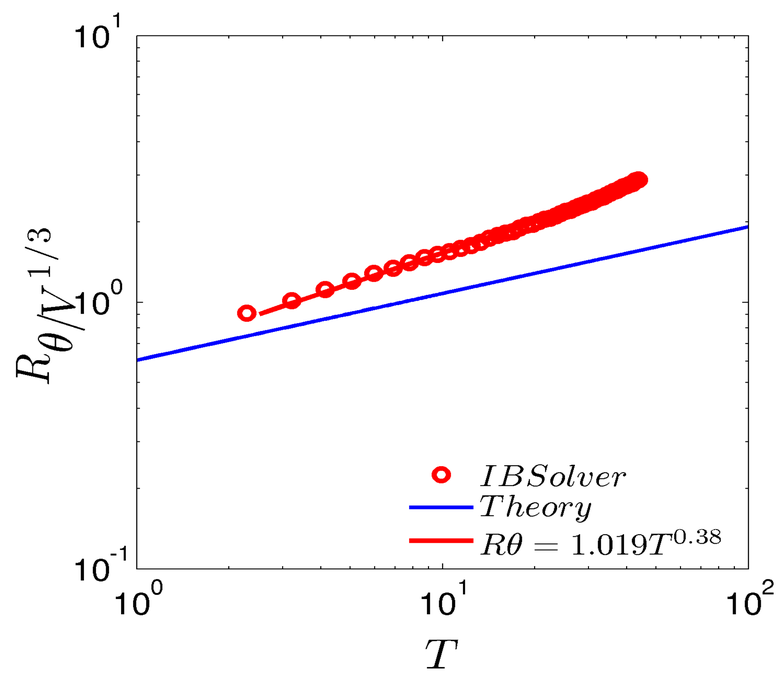


Fig. 2: Non-dimensional average flow length of a deformed droplet on top of a sphere as a function of non-dimensional time (dimensionless parameters same as in Fig. 1)

Conclusions and Outlook

DNS prediction of the gas-liquid-particle multiphase flow have been carried out for thin film spreading on a spherical substrate. The accurate of the DNS solver has been studied as a function of the grid spacing, and we find that extremely fine grid are required to keep the loss in acceptable limit. The simulation results for the liquid spreading rate indicate only a fair agreement with lubrication theory [1], which is valid for the limit of zero Reynolds number (i.e., in the absence of inertia). The difference between the numerical simulation and the theory is due to the different Bond numbers considered. Future work is required to better understand the effect if the fluid inertia, as well as that of the Bond number Bo_V .

Acknowledgement

We acknowledge the funding of the FWF through project P23617 and we gratefully acknowledge support from NAWI Graz by providing access to dcluster.tugraz.at.

Notation

$\vec{u}$	Fluid velocity $[m/s]$	μ_g	Viscosity of gas $[kg/(m\cdot s)]$
p	Pressure $[N/m^2]$	R	Radius of the sphere $[m]$
ρ	Fluid density $[kg/m^3]$	V	Initial volume of the droplet $[m^3]$
$\vec{f}_s$	Acceleration by surface tension force $[m^2/s]$	γ	Surface tension $[N\cdot m^{-1}]$
$\vec{f}_p$	Acceleration by fluid-particle interaction force $[m^2/s]$	T_{ref}	Reference time scale $T_{ref} = v_l R / gV^{2/3}$
$\vec{g}$	Gravitational acceleration $[m^2/s]$	Bo_V	Bond number $Bo_V = (\rho_l g V)/(\gamma R)$
ρ_l	Density of liquid $[kg/m^3]$	Re	Reynolds number $Re = (\gamma R)/(\rho_l v_l^2)$
ρ_g	Density of gas $[kg/m^3]$		
μ_f	Viscosity of liquid $[kg/(m\cdot s)]$		

References

[1] D. Takagi and Herbert E. Huppert, Journal of Fluid Mechanics 647 (2010).

[2] Huppert, H. E, Nature 300 (1982).

Contact Details
Ass.Prof. Dr.techn. Dipl-Ing. Stefan Radl
Assistant Professor, Simulation Science Group
radl@tugraz.at - ippt.tugraz.at