Modeling Solid-Liquid Settling System as a Two-Phase Flow Problem

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Abstract

A challenging two-phase flow problem is modelled and simulated in COMSOL Multiphysics environment. Velocities of a single solid bead settling in different liquids are determined by the simulation and compared to measurement value. Fluid-solid interaction is approached by Level Set interface tracking method with the cost of treating solid as a viscous fluid. Method parameters are examined and found to be a good tool in modeling sedimentation. The study is ready to be continued by other modelling approaches.

Keywords: CFD, two-phase flow, solid-fluid system, sedimentation

Introduction

Sedimentation is a challenging two-phase problem to model and simulate.[1] Many applications in the industry use sedimentation for separation. For example treatment of wastewater often carried out in settling basins. Different types of the sedimentation process include independent and zone settling. The food industry uses the sedimentation process as well. Most dairy products made by separate dense parts of milk out of less dense leftover. A device for sedimentation can be equipped by a rotating motor which enhances the effect of gravitation via centrifugal force. However in milk and cheese industry both the continuous and the disperse phases are liquid, the same model can be applied to the liquid-solid system by varying the properties of the second fluid (dispersed phase).

Computational Fluid Dynamics is a quickly spreading tool to calculate and simulate flow fields as even normal PC's computing capacity grows. Computers can efficiently solve partial differential equations such as the Navier-Stokes equation. In the case of a two-phase system, the interaction between the phases modifies the flow patterns. There are several modeling approaches to handle solid-fluid problems. Two-fluid method (TFM) or Euler-Euler method treats both phases as a fluid even when one of them is a solid phase. Discrete element method (DEM) is a modelling approach which results in detailed information about each element of the solid phase. However, its computational cost is high. Both earlier mentioned methods use approximately one order of magnitude larger mesh than the size of a typical particle of the solid phase. Direct numeric simulation techniques work in contrast one order of magnitude smaller mesh to calculate the flow field, and the replacement of the solid particles.[2] Two main subtypes of this method is the one which uses body-fitted mesh, and the other which use regular Cartesian time-independent mesh. By use of body-fitted mesh, the particles occur as a boundary or wall, while by the use of the other subtype, a so-called immersed boundary takes place where the particle occurs only virtually without a physical boundary. This makes the method computationally reasonable, while we have to face other kinds of challenges by using immersed boundary-type methods, for example how to define the connection between the node points of the fluid and the solid.[3] In the case of body-fitted mesh it is not an issue. However there are other types of difficulties. As the particle is defined by a boundary, every replacement changes the geometry of the computational field, which means the mesh changes in every time-step. Projection of flow field properties between the old node points and the new ones is not trivial either. Arbitrary Lagrangian-Eulerian (ALE) technique is one good approach to solve this problem, and moving mesh models are based on ALE.[4]

CFD module of COMSOL Multiphysics offers opportunities to handle immiscible phases. Disperse methods include bubbly flow, mixture model and Euler-Euler model, however bubbly flow can handle only bubbles as a dispersed phase and thus is improper for sedimentation. All these three disperse methods roots in the first (Euler-Euler) method. It could be applied to model the movement of a crowd of particles in a fluid. On the other hand, interface tracking methods are more resolved thus able to model individual particles as well as interfacing phases. Level set and phase field approaches beside of moving mesh method seem more appropriate than the Euler-Euler method for the single bead settling purpose.[5] These approaches are interface tracking methods, which mean that the interface between two immiscible fluids is tracked by a color function or an auxiliary function on a fixed mesh in the first two approaches, and tracking the interface position with a moving mesh in the latter approach. Phase-field method is under high research interest nowadays too; a meshless approach is introduced in a recent paper.[6]

2D axisymmetric model can be used as a good and computationally economic approximation of the real 3D system. As a starting point, we opened the rising bubble model from COMSOL's Application Library. After studying this example, we tailored it to our needs. Solid dispersed phase is treated as a liquid with high viscosity to imitate solid behavior while keeping the ability to use the same flow equation by solving an additional transport equation. Level set and phase field methods use fixed mesh, and the difference of the properties of the two phases at the interface is described by a step-like color function. Moving mesh method gives an alternative way to model two-phase flows with importance to interface tracking. In this study, as a first round, Level Set method is used to find out how can COMSOL Multiphysics help in the task of settling individual particles in a given liquid.

Model Set-up

In our model 5.9 mm sphere shaped solid particles are dropped into a 100 mm diameter and 400 mm high column of liquid (water, silicone oil, paraffin oil or gear oil). The aim of the simulation is to predict the settling velocity of the particles. The properties which influence the settling can also be explored by modeling. The built CFD models will be validated by experimental measurements in the near future. One measurement result is available for us which gave the terminal velocity of the nylon bead in water to 143 mm/s. Figure 1 shows the geometry of the experimental set-up.

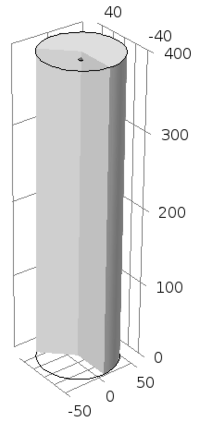

Figure 1. The geometry of the equipment with the bead [mm]

The model is built for the same geometry and is used for the simulations too, however for gaining more reasonable solution time, the geometry of the vessel is reduced in some cases.

Governing Equations

According to Stokes law, the excepted velocity can be calculated by the forces acting on the immersed body. Newton's second law of motion says that the acceleration of a body is caused by the sum of all forces acting on the body. As we are interested in the terminal velocity, the case when acceleration has already become zero should be described (Eq.(1)).

$$mg - F_{buoyancy} - F_{drag} = 0 \qquad (1)$$

where m is the mass of the bead, g is the gravity acceleration constant, $F_{buoyancy}$ is buoyancy force and F_{drag} is drag force. Buoyancy force equals to the weight of a same volume fluid as the immersed solid (Eq.(2)).

$$F_{buoyancy} = \rho_{fluid} \cdot V_{solid} \cdot g \qquad (2)$$

where ρ_{fluid} is the density of the fluid and V_{solid} is the volume of the immersed solid body. Drag force depends on the quality of fluid, the shape of the immersed solid body and its terminal velocity (Eq.(3)).

$$F_{drag} = \frac{1}{2}\rho_{fluid} \cdot u^2 \cdot c_D \cdot A \qquad (3)$$

where u is the velocity of the bead c_D is the drag coefficient which is a shape dependent dimensionless number, in case of sphere is 0.47 and A is the reference area. By sorting Eq(1), u can be determined (Eq(4)).

$$u = \sqrt{\frac{2\cdot(\rho_{solid} - \rho_{fluid})\cdot V_{solid}\cdot g}{2\rho_{fluid}\cdot c_D \cdot A}} \qquad (4)$$

Reynolds number is a dimensionless number which gives an insight into the quality of the flow in terms of linear or turbulent regimes. Re can be calculated by Eq.(5).

$$Re = \frac{\rho u L}{\mu} \qquad (5)$$

where ρ is the density of the fluid, u is the velocity of the fluid with respect to the object, L is a characteristic length, μ is the dynamic viscosity of the fluid. A flow can be considered as laminar flow if the Reynolds number is under 2000.

Materials and Methods

Table 1 summarizes the important physical properties of the examined phase materials.

Table 1: Properties of the two phases

	Density (kg/m^3)	Dynamic viscosity (Pas)	Volume (m^3)	Temp. (°C)
nylon	1114	"10"	1.08*10^{-7}	25
water	1000	0.0009	0.04	25
silicone oil	1000	0.6	0.04	25
paraffin oil	827-890	0.11-0.23	0.04	25
gear oil	850	0.32	0.04	25

COMSOL Multiphysics is used to simulate the settling of a single solid sphere in different fluids. Out of COMSOL's two-phase modeling tools, Level Set method is chosen as it can track the interface between phases properly. Laminar flow is chosen as physics as the Reynolds number, in this case, is under 2000. In our case, it is around 140 if we count by one-tenth of the vessel diameter as a characteristic length. The physical model of the laminar single-phase flow is incompressible as we do not model gas phase this time at all. Gravity is included with the built-in gravity acceleration constant. Multiphysics coupling option is set to Level Set method, the reference pressure level is 1 atm, the temperature is 298.15 K (25 °C). Initial values are 0 m/s velocity in all directions. As the used geometry is 2 dimensional axisymmetric, axial symmetry should be given to the middle boundary. At the outer walls, no-slip boundary condition is defined. A pressure point constraint is given for the circle as 0 Pa and to compensate for hydrostatic pressure. The time-dependent form of the equations used by Laminar Flow module are the momentum equation (Eq.(6)) and the continuity equation (Eq.(7)).

$$\rho\frac{\partial u}{\partial t}+\rho(u\cdot\nabla)u=$$

$$\nabla\cdot[-pI+\mu(\nabla u+(\nabla u)^T)]+F+\rho g \qquad (6)$$

$$\rho\nabla\cdot(u)=0 \qquad (7)$$

where p is the pressure, I is the identity matrix.

The interface was tracked by Level Set method (Eq.(8)).

$$\frac{\partial\Phi}{\partial t}+u\cdot\nabla\Phi=$$

$$\gamma\nabla\cdot\left(\epsilon_{ls}\nabla\Phi-\Phi(1-\Phi)\frac{\nabla\Phi}{|\nabla\Phi|}\right) \qquad (8)$$

where Φ is the level set function, it is between 0 and 1 depending on the phases (0 is for Fluid 1, 1 is for Fluid 2 and 0.5 means the interface), γ is the reinitialization parameter, which should be set to the order of magnitude of the expected interface velocity (0.1 m/s in this case), ε_{ls} is the parameter controlling interface thickness. The initial interface is the boundaries of the sphere.

The Component's Multiphysics branch sets the details of the two-phase flow. As level set method works for two immiscible liquid phases or liquid and gas phases, all materials are treated as fluids. Thus Fluid 1 in our case is the solid bead with a user-defined density of 1114 kg/m^3 and dynamic viscosity of 10 Pas. Fluid 2 is the environment liquid with different properties according to Table 1. Surface tension is neglected in the momentum equation.

User-controlled mesh is chosen with a maximum element size of the one-tenth of the bead diameter. This builds free triangular as Figure 2 shows.

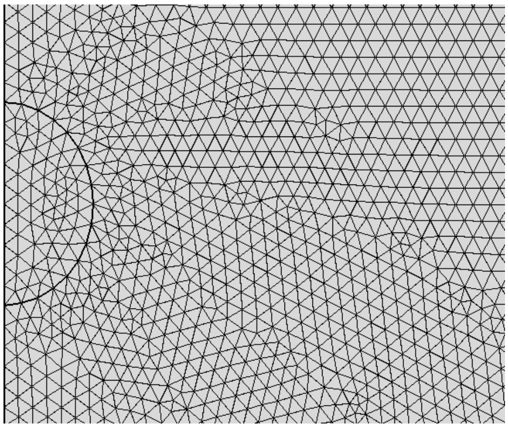

Figure 2. Mesh elements near the interface of the two phases

These settings result 150246 domain elements and 1542 boundary elements for the whole geometry. Mesh dependency study has not taken for the meshing is carried out by following a rule of thumb suggested by COMSOL support in Two-Phase Flow Modeling Guidelines. Maximum mesh element size in all domains is set to one-tenth of the bead.

Simulation Results and Discussion

The used model is examined by changing density and surface tension parameters in case of only one chosen Fluid 2 material. A bead (Fluid 1) with different density values are placed in the water-filled tank, and resulted velocities are compared to measured value (Table 2, Figure 3). In these investigations reduced geometry is used to decrease computational time. The diameter of the reduced vessel is 25 mm (a quarter of the original), height is 200 mm (half of the original), and the diameter of the bead does not change. Simulations are run in COMSOL Multiphysics environment on a PC with 16 GB RAM and an Intel Core i5 CPU with 2.66 GHz.

Table 2: Different density values for Fluid 1, and velocities resulted by level set interface tracking

Fluid	**Density [kg/m^3]**	**u [m/s]**
Water	1000	0.0421
Fluid 1	1150	0.0765
	1500	0.1081
	2000	0.133
	2500	0.1491
	2700	0.0421

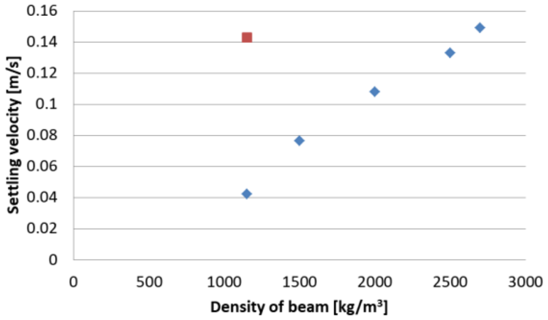

Figure 3.Settling velocities of different density bead (blue diamond) and the measured velocity (red square)

For changing the density of material changes the material itself, further investigations are neglected in this direction. On the other hand, we examined the effect of changing the surface tension parameter (Table 3, Figure 4). A material with 1150 kg/m^3 density is chosen for Fluid 1 and water for Fluid 2.

Table 3: Surface tension coefficients and the velocity differences from the measured velocity

Surface tension coefficient [N/m]	u_{diff} [m/s]
0.01	0.1012
0.5	0.1027
1	0.1027
1.5	0.1029
2	0.1032
2.5	0.1032
3	0.1035

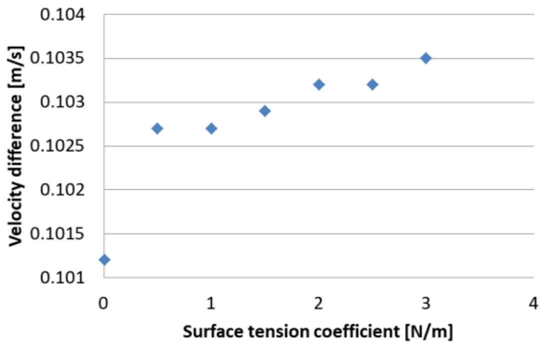

Figure 4.Effect of surface tension coefficient on the error of the simulation compared to the measurement

As the velocity difference is lower in case of lower surface tension coefficients, further simulations are taken by low surface tension coefficients or even by neglect surface tension.

After the model investigations, we turned to a material study, i.e. how does the same nylon bead settle in different fluids. Reduced geometry is used by the methods introduced in Material and Methods chapter for sensitivity analysis of the model parameters. Diameter of the new vessel is 25 mm, height remained 400 mm, and the size of the bead does not change either. This gives much less elements, 18279 domain and 999 boundary elements, thus less computational time. Time-dependent studies are computed for 6 seconds with 0.2 s time step. Solution times and settling velocities for nylon bead in different fluids are summarized in Table 4. Velocity fields after 6 s is observable in Figure 5.

Table 4: Results of simulation for terminal velocity and their solution times

Fluid	Solution time [s]	u [m/s]
water	5236	0.0463
silicone oil	318	0.0043
paraffin oil 1	3073	0.0175
paraffin oil 2	2181	0.0086
gear oil	1846	0.008

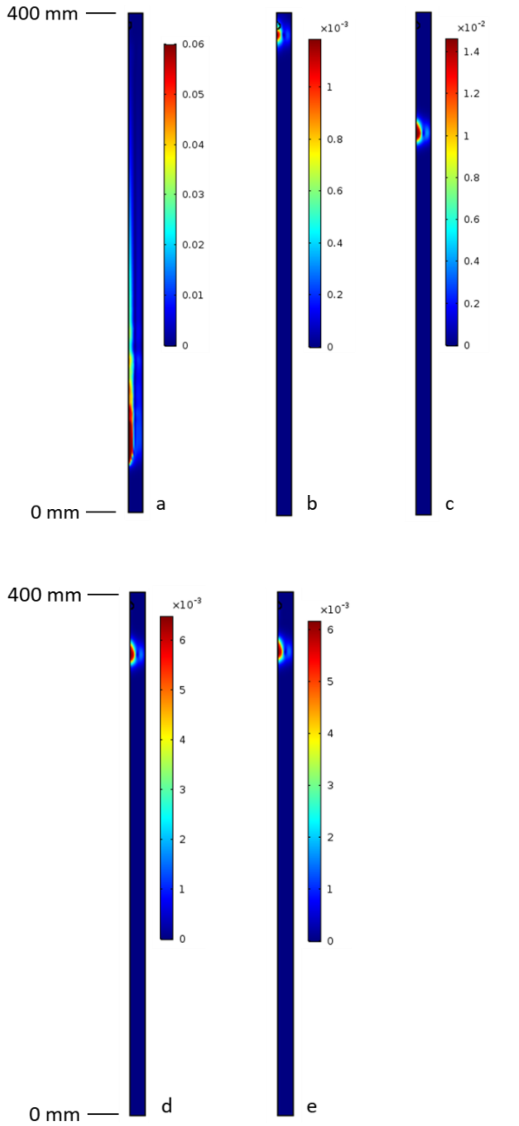

Figure 5. Velocity fields [m/s] in case of the different fluids. a) water, b) silicone oil, c) paraffin oil 1, d) paraffin oil 2, e) gear oil

Right after 2 seconds, noticeable deformation occurs in each case (Figure 6). This could be caused by the improper choice of dynamic viscosity of the quasi-solid material. In all examined fluids, nylon bead got 10 Pas as a user-defined dynamic viscosity value. In water it worked relatively well but probably in other, more viscous materials it should have been set higher too.

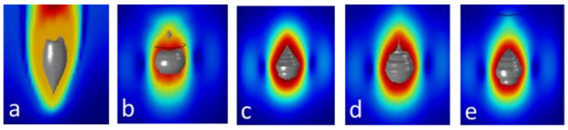

Figure 6. Deformation due to treating solid bead as a viscous fluid in different environments. a) water, b) silicone oil, c) paraffin oil 1, d) paraffin oil 2, e) gear oil

Deformation, as well as velocity, depends on viscosity and density too. Table 5 contains the calculated velocities in case of different environments (different Fluid 2 materials, see their properties in Table 1).

Table 5: Velocities in dependence of density (y-axis) and viscosity (x-axis)

	0.0009	**0.11**	**0.23**	**0.32**	**0.6**
1000	0.0463				0.0043
890			0.0086		
850				0.008	
827		0.0175			

According to the simulated velocity results, two diagrams can be drawn on depending on the density and the dynamic viscosity of the fluid (Figure 7).

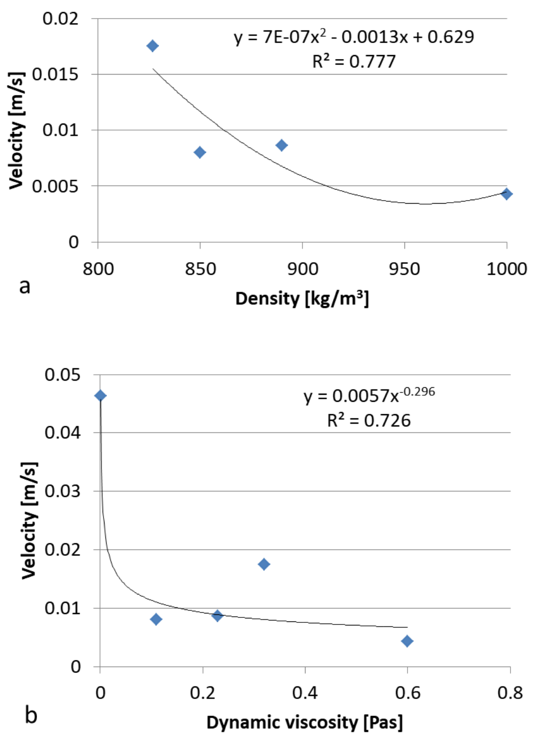

Figure 7. Diagrams of the density (a) and viscosity (b) dependence of velocity

Based on the curve fitting an expression is defined to include the changes from density and viscosity as well (Eq 9). A global nonlinear optimization algorithm (NOMAD) is used to identify the parameters 1 to 5 of the curves describing the correlation.

$$v=par(1)*\rho^2+par(2)*\rho+par(3)*\nu^{par(4)}+par(5) \quad (9)$$

The objective function of the optimization algorithm is to minimize the difference of the velocity where we have values in a 2D plane. The process results the best parameters as the followings 1e-7, -2e-4, 1e-3, -0.5, 0.1 respectively. A color map diagram made based on the resulted bead velocity plane depended on fluid density and fluid viscosity (Figure 8).

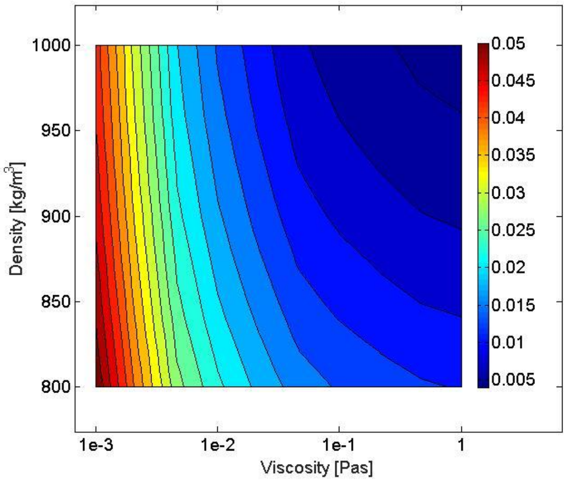

Figure 8.Velocity [m/s] as a color map in dependency of density and viscosity of Fluid 2

Higher viscosity makes the bead settling velocity lower, and the same correlation can be observed by fluid density too, i.e. in lower density fluid the buoyancy force became lower thus the sum of forces is higher in the positive direction (downward).

Conclusions

Simulation result of the modelled sedimentation tank is calculated for model investigations and to calculate terminal velocities of a single 5.9 mm diameter nylon bead in different fluids. A 0.1 m diameter and 0.4 m high cylinder is filled with water, silicone oil, paraffin oil or gear oil. A time-dependent study by COMSOL Multiphysics CDF Module Laminar flow field and Level Set Multiphase model is ran, and velocity of nylon bead is determined from the simulation. Velocities are compared and falling nylon bead in water has found as the highest velocity of 46 mm/s. This result fits into expectation as a correlation has been discovered by seeking a relation between density and velocity, and viscosity and velocity. Interpolation has shown that in less dense liquid the settling is faster and also in more viscous fluid the settling is slower. However the velocity tracked by the model does not reach the measured value, deeper understanding the model and its proper parameter setting could help to gain better similarity.

The used numerical two-phase flow interface tracking method can be applied to fluid-fluid or fluid-gas systems, although we use it to model the solid-fluid system. The solid phase is defined by a viscous fluid, and thus its original sphere shape deforms by the other fluid around it. Further parameter tuning could improve the results to make the simulations more realistic. COMSOL's Moving Mesh method will be the next tool to model the settling system. We have already some result from using the Moving Mesh method, however deeper understanding of the method is needed to continue the modeling work in this direction. The built CFD models will be validated by experimental measurements. As another type of model validation, the theoretic equations should be extended by a term which includes the effect of viscosity as well. After this, comparing the simulated results with analytical results can serve as a second validation.

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