Calculation task 1 – Multiphase flow course

Task 1.1: 1-D simulation of a spherical glass particle settling in water

Background and general description

In this task we deal with the settling of a **particle A** in an infinitely long channel filled with water (density: 1000 kg/m^3) at 20□C. The particle A has the following properties:

Table 1 - Particle A properties

Properties of particle A	
Diameter	0.5 mm
Density	2560 kg/m^3

The cumulative effect of the forces acting on the particle A (namely: the drag, buoyancy and gravity effects) is responsible for the observed settling. After some time (or length traversed along the channel) the particle A attains a constant velocity, termed the *terminal velocity of settling*, as a consequence of the net balance of forces acting on it. This settling velocity is one of the key variables in multiphase flow systems involving sediment transport and it is critical to our understanding of suspension formation, deposition and mixing.

In the current task you will simulate the settling of a spherical glass particle (as described in Table 1) in an infinite channel filled with water, using your own solver (i.e. not a commercial CFD code) developed using any of the available tools (Matlab, Mathematica, Python, C++, R script etc.).

Numerical details (discretization)

The fundamental idea behind such a solver is the solving of Newton's second law of motion for the particle at every relevant time step. You are supposed to formulate the relevant force balance around the particle and solve the equation below:

$$m_p \frac{dV_p}{dt} = F_{total}, \tag{1}$$

where m_p and V_p are the particle mass and velocity, respectively, and F_{total} is the sum of all relevant forces acting on the particle. A simplest method for solving Equation 1 is the *Forward Euler Method (FWE).* The *FWE* uses the definition of the derivative of a function *y(t)* at a point *t*. This is done as follows:

- if we first recall the definition of a differential from calculus,

$$\frac{dy}{dt} = \lim_{h \to 0} \frac{y(t+h) - y(t)}{h} \tag{2}$$

- an approximation for expression 2 can be obtained by setting $h = \Delta t$ and $t = t_0$ (the initial state).

This would lead to:

$$\frac{dy}{dt} \approx \frac{y(t_0 + \Delta t) - y(t_0)}{\Delta t} \tag{3}$$

where Δt is any relevant step length (or interval length). To write a difference expression for expression 3 we let Y_i denote our approximation to $y(t_i)$; clearly $Y_0 = y(t_0)$ which is the initial condition. We can then obtain expression 4, which is understood as the general form of the *FWE* method.

$$\frac{Y_1 - Y_0}{\Delta t} \approx f(t_0, Y_0) \tag{4}$$

By having the value of a function at a previous state (t_0), we can approximate its value at the next state ($t_0 + \Delta t$) using the rewritten form of expression 4:

$$V_{p_1} \approx V_{p_0} + \Delta t \frac{F_{total}(t_0, V_{p_0})}{m_p} \tag{5}$$

where, V_{P0} and V_{P1} are the particle velocities at times $t = t_0$ and $t = t_0 + \Delta t$, respectively.

Additionally, expression 5 can also be derived by using a truncated Taylor series expansion, and consequently an error referred to as the *local truncation error is* induced at every time-step of the method. For the *FWE* method it can be shown that this error is of the order $O(h^2)$ and hence the method is referred to as a *first order* technique. Another important observation regarding the *FWE* method is that it is an *explicit* method, i.e., y_{n+1} is given explicitly in terms of known quantities such as y_n and $f(y_n,t_n)$. Explicit methods are easy to implement; however, the drawback is in the limitation of the time step size to ensure *numerical stability*. Keep this in mind while choosing your time steps.

Assumptions

Note that the given task can be solved to a varying degree of accuracy. To have a more uniform set of results, you are encouraged to incorporate the following assumptions:

1) Assume that the particle starts from rest, $V_p(t = 0) = 0$
2) Additionally, let the particle settle only along the positive z-direction (starting at $z = 0$). Use the uploaded experimental data (ExptData.dat) to guess a relevant terminal velocity for the settling particle. This guess would aid you calculate the relevant particle Reynolds number.
3) Assume an appropriate drag law for the settling sphere
4) Assume that water in the channel is not disturbed extensively by the settling particle ($U_{water} = 0$)
5) '***g***' acts in the negative z direction.

Questions to be discussed

Q1) how can we define the particle response time (τ_p)? Calculate τ_p for your simulation. What is the effect of changing the particle/fluid density ratio on τ_p? Explain your results with a plot of τ_p vs. the density ratio.

Q2) what is the Stokes number (*St*) of the particle A? Hint: assume a suitable macroscopic length and time scale for the fluid. Explain the importance of *St* to determine the order of coupling required between the fluid and particulate phases in sedimentation transport. Is the one-way coupling between the particle A and water described in Task 1.1a reasonable enough approximation for the flow physics? Explain.

Q3) plot the evolution of the terminal settling velocity for the particle A. Compare your results with the provided experimental data in the course homepage. Does your 1-D solver compare well with the experimental measurements? Explain the observed comparison trends.

Q4) an expression sometimes used to calculate the drag coefficient C_D is:

$$C_D = \frac{1}{2} + \frac{24}{Re_p}$$

Calculate the terminal settling velocity for the particle using the expression above. How does it differ from the profile calculated in Q3? For how long will the particle accelerate?

Q5) simulate a case for the particle A settling in air at 20□C.

i. Compare this result (use relevant plots!) with the trends noted in Q3. Discuss the key differences noted.
ii. What is the particle response time for such a simulation? Would the assumptions made while setting up the *FWE solver* continue to be valid? Explain.

Q6) Repeat Q3 (particle A settling in water) using a higher order explicit or implicit scheme (for e.g. Improved Euler scheme or another scheme). What changes do you note? Discuss with relevant plots.

Task 1.2: 1-D simulation of an ellipsoidal air bubble rising in water

Background and general description

The formation of gas bubbles and their subsequent rise due to buoyancy are fundamental phenomena that have a great impact on the hydrodynamics of gas-liquid reactors. Most commonly, the formation of bubbles is achieved either by automation of liquid into gas in the form of drops or by bubbling (sparging) of gas into the liquid. Several common operations in the chemical process industry, petrochemical industry, and mineral processing are designed based on the knowledge of the hydrodynamic parameters suitable for a desired performance.

It is known that bubbles in the diameter range of 0.1–0.2 cm rising in clean water are ellipsoidal in shape. Additionally, the bubble path is rectilinear when the equivalent diameter is less than about 0.13–0.18 cm [1]. In the current task you are required to simulate a rising ellipsoidal air bubble (as described above) in an infinite channel filled with water, by extending the solver developed in Task 1.1. Assume an equivalent bubble diameter of 0.15 cm for this task.

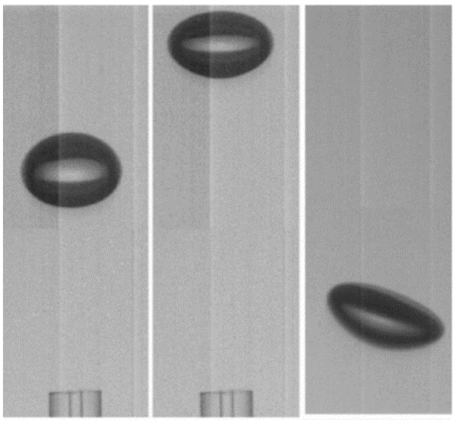

Figure 1- Typical examples of ellipsoidal bubbles (captured in experiments).

Questions to be discussed

Q7) state all the relevant assumptions that you would employ to simulate Task 1.2. Motivate them.

Q8) what is the τ_p for this case? How does it differ from that of a spherical air bubble and why?

Q9) plot the evolution of the terminal rise velocity of the ellipsoidal air bubble. (Hint: Estimate the drag on the ellipsoidal bubble using shape factors). What happens to the rise velocity if water is replaced by oil?

Q10) what is the Weber number of the given bubble and how would it effect the bubble rise velocity? Explain.

Q11) what is the Marangoni effect? How would it affect the bubble movement? Discuss the conditions under which this effect can be ignored. Explain.

References

1. Wu, M. and M. Gharib, *Experimental studies on the shape and path of small air bubbles rising in clean water.* Physics of Fluids, 2002. **14**(7): p. L49-L52.