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I2 Report

An Investigation into MULES and its Application into Simulating Settling Behaviour in an Armfield Rectangular Settling Tank

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4th year MEng Group Project

I certify that all material in this thesis that is not my own work has been identified and that no material has been included for which a degree has previously been conferred on me.

Signed..

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I2 Report

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Abstract

Multiphase simulations to show the flow regime of a rectangular settling tank and settling tube are presented. The simulations, performed using driftFluxFoam on the open source software, OpenFOAM, model secondary sludge, Olive Stone Powder and a combination of the two. The results of the simulations indicate that Olive Stone Powder is not a suitable sludge substitute with regards to wastewater modelling.

Keywords: OpenFOAM, Multiphase, Olive Stone Powder, Computational Fluid Dynamics, MULES, Phase Fraction

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1. Introduction and Background

1.1. *Hydro International*

Hydro International are a company who “provide advanced products, services and expertise to help municipal, industrial and construction customers to improve their water management processes, increase operational performances and reduce environmental impact” [1]. They’ve been operating on a global scale since the 1980s and function effectively as a business, having a revenue of £37.9 million and adjusted profit before tax of £2.4 million [2].

Hydro issued the team with an IP agreement containing key deliverables. Two of these deliverables were to perform simulations on both the rectangular sedimentation tank and vortex separator and to compare the results of the simulations with empirical data. In addition to this, the settling velocity of Olive Stone Powder should be determined. This report addresses the simulation of the rectangular sedimentation tank and the simulation of the experimental methods used to determine settling velocity.

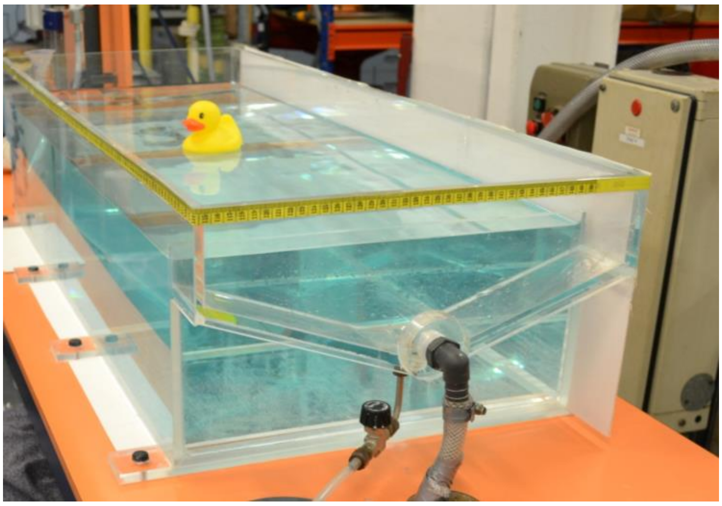

Figure 1: Armfield Rectangular Tank

1.2. *OpenFOAM*

OpenFOAM (Open Field Operation And Manipulation) is a free, open source software used for implementing techniques of Computational Fluid Dynamics (CFD). The software was released and heavily worked on by OpenCFD Ltd in 2004. OpenFOAM allows the user to simulate scenarios involving fluids to determine properties of fluid flow. Using OpenFOAM is similar to using commercial CFD software in the sense that the user goes through pre-processing, meshing, solving and post-processing. It is, however, very different in that it trades the standard Graphical User Interface for greater possibilities with respect to possible solution algorithms and allows for the user to implement their own code into OpenFOAM [3].

1.3. Aims

The aim of this project is to assess the functionality of the Armfield rectangular tank through the use of CFD techniques. Doing so will provide an insight as to how the tank performs and how Olive Stone Powder (OSP) can be used as a substitute to sludge in the wastewater industry, specifically for Hydro International. In addition to this, the project aims to compare and validate the properties of OSP calculated through experiments computationally.

1.4. Objectives

- Study the previous work carried out on settling tubes and the rectangular sedimentation tank through a literature review.
- Study how to perform multiphase simulations and observe what techniques are available. This should include an in-depth study of MULES (Multidimensional Universal Limiter of Explicit Solutions).
- Create a suitable mesh for a settling tube.
- Perform a mesh refinement study for the settling tube.
- Implement the previously studied multiphase modelling techniques on both the settling tube mesh and a provided mesh for the Armfield rectangular tank.
- Analyse the performance of each and compare the computational results to the experimental team's results. The results should be used to either validate or invalidate the use of OSP as a sludge substitute.

2. Literature Review

2.1. Settling Tubes

A settling tube, otherwise known as a settling column or settling velocity tube, is a vertical, cylindrical column in which settling is observed. The cylinder is typically filled with fluid containing dispersed solid particles. Over time, the particles are observed to sink to the bottom of the tube with an interface between the two phases. This is covered in greater detail in Wye's report, [4]

In 1971, a paper was produced by Gibbs, Matthews and Link which found 'The Relationship between Sphere Size and Settling Velocity', [5]. This report aimed to measure the settling velocity of 216 glass spheres of varying diameters and this was achieved with a 95% confidence level. This study found an equation to approximate the settling velocity from sphere size:

$$V = \frac{-3\eta + \sqrt{9\eta^2 + gr^2P_f\left(P_s - P_f\right)(0.015476 + 0.19841r)}}{P_f(0.011607 + 0.14881r)} \tag{1}$$

where V is settling velocity, η is the dynamic viscosity, g is the acceleration due to gravity, r is the sphere's radius, P_f is the density of the fluid and P_s is the density of the sphere.

This equation provided an excellent agreement with observed data as there was less than a 2.5% difference between their calculated values and the observations for all 216 spheres.

20 years later, in 1991, concepts of settling velocity and the thickening process of suspended solids was discussed by Takacs, Patry and Nolasco in their paper 'A Dynamic Model of the Clarification-Thickening Process', [6]. This paper provided a model which aimed to predict the solids profile through the settling tube. The paper also provided an equation which defined the settling velocity in the cylinders by exponentials.

$$V = v_0e^{-r_hX_j^*} - v_0e^{-r_pX_j^*} \tag{2}$$

where v_0 is the maximum settling velocity, r_h is the settling parameter characteristic of the hindered settling zone, r_p is the settling parameter characteristic of low solids concentration and X_j^* is the difference between the suspended solids concentration and the minimum attainable suspended solids concentration.

The model was used to compare data between pilot and full-scale experiments with good results. The report itself goes into depth about the mathematics involved in the calculation and importance of the calculation of settling velocity. Additionally, there is much detail regarding settling models which had been conceived prior to this paper and how these related to the model created in the paper.

2.2. Rectangular Tanks

The concepts from settling tubes and settling velocity are essential when considering rectangular settling tanks. A 1992 report, 'Modelling of Rectangular Settling Tanks' from Zhou and McCorquodale, [7] presented a model to predict the velocity field in a rectangular tank. The presented model correctly predicted the general shape of the flow field, including "a well-developed bottom current and a counter flow in the upper region of the settling zone". This paper also suggests that the high entrainment in the "influent plume" can be reduced by a baffle located past the inlet.

The Zhou and McCorquodale paper provided details of the velocity profile, however did not discuss observations in settling to the same extent. Insight of this can be found in the 1998 work from Mazzolani, Pirozzi and d'Antonoi (Mazzolani et al) [8]. This report compares the use of three settling models applied to a rectangular tank: the DSM, the MSM and the GSM. The DSM relates the particle diameter to the overall settling velocity. The MSM is brought forward from the 1991 works of Takacs et al, [6]. Finally, the GSM "accounts for both different particle velocities in discrete settling conditions and particle interactions in hindered settling conditions". These models all gave reasonable predictions of the hydrodynamic field for the case which were all "qualitatively similar". This report establishes that it's required that more research is undertaken in this area such that solid transport modelling in sedimentation tanks can be improved.

2.3. Multiphase Flow Techniques

A 2011 article from Raeini, Blunt and Bijeljic showed how the Volume-Of-Fluid method can be used to model a two-phase flow [9]. This paper explains how the Navier-Stokes equations (which are central to their porous media multiphase flow problem) can be discretised using a finite volume approach and the Volume-Of-Fluid method can subsequently be used to realise the interface location.

The numerical method is described in detail throughout the paper: it begins with the discretisation of interface curvature by use of interpolation and a Gauss scheme. Following this, the capillary forces are discretised by calculating them at face centres and an indicator function is used. Once the discretisation and linearisation occurs, the momentum equations can be written, pressure and velocity get coupled and the pressure and velocity can be iteratively solved for. This requires use of the PISO (Pressure Implicit with Splitting of Operators) algorithm.

Particularly relevant to this project was Daniel Brennan's 2001 Thesis (submitted for the degree of Doctor of Philosophy of the University of London) [10]. This project, titled 'The Numerical Simulation of Two-Phase Flows in Settling Tanks', "describes the development and application of a mathematical model of the two-phase flow regime found in settling tanks used in the activated sludge process".

This paper covered many important aspects of two-phase modelling in the context of settling tanks. Early on in the report, Brennan discusses the use and types of settling tanks before going into detail about the settling process and how settling velocity is an important factor. There is a great detail of the mathematics of the settling velocity and in addition to this, how the rheology of the system influences the overall flow regime. There is discussion of single phase computational models (including Finite Element Methods and the standard k-ε model) used in settling tanks which leads into the more important, dispersed phase transport models. This section provided a historical look at the development of dispersed phase models.

The following chapter, "Mathematical Formulation of Two-Phase Flow", discussed the mathematics of the Drift Flux model and other Eulerian methods (Lagrangian approaches were deemed inappropriate for settling tank modelling). After a discussion of turbulence, the report moved towards the performed simulations.

The report included both two-dimensional and three-dimensional simulations on the rectangular settling tank. Both types of simulation produced velocity and phase fraction profiles through use of the Drift Flux Equations and the PISO algorithm.

Brennan’s work was said to produce “good accuracy in all cases” and generally includes a large amount of useful information which can be applied to many multiphase cases requiring Drift Flux. His work is especially important for the application of multiphase techniques to settling tanks and the activated sludge process [10].

3. Theoretical Background

3.1. Multiphase Flow

A flow containing more than one phase is known as multiphase. This could consist of bubbles/particles dispersed in a fluid or the combination of two or more immiscible fluids. Each phase involved in the flow is given a value for phase fraction (denoted as α) which represents what proportion of the mixture is that substance. For a two-phase mixture in a model, each cell has a phase fraction total of 1:

$$\alpha_1 + \alpha_2 = 1 \tag{3}$$

3.2. Volume-Of-Fluid Method

Volume-Of-Fluid (VOF) method is a Eulerian practice: it treats all phases as continua rather than tracking the location of individual particles (Lagrangian). For simulations with a large number of dispersed particles, using Eulerian schemes over Lagrangian saves on computational time [11].

For the VOF Method, the required momentum equations are given by:

$$\nabla . \boldsymbol{U} = 0 \tag{4}$$

$$\frac{\partial \alpha}{\partial t} + \nabla . (\boldsymbol{U}\alpha) = 0 \tag{5}$$

$$\frac{\partial (\rho \boldsymbol{U})}{\partial t} + \nabla . (\rho \boldsymbol{U}\boldsymbol{U}) = -\nabla p + \nabla . \boldsymbol{T} + \rho f_b \tag{6}$$

where **U** defines the velocity field, α is the phase fraction, ρ is the density, p is the pressure, **T** is the deviatoric viscous stress tensor and f_b is the body force per unit mass [12].

For a Eulerian model containing two fluids (1 and 2), the following two equations can be expressed:

$$\frac{\partial \alpha}{\partial t} + \nabla.(\boldsymbol{U_1}\alpha) = 0 \quad (7)$$

$$\frac{\partial (1-\alpha)}{\partial t} + \nabla.[\boldsymbol{U_2}(1-\alpha)] = 0 \quad (8)$$

A 'compression velocity', otherwise known as the relative velocity, can be introduced and this allows for the arrangement of an 'evolution equation' of phase fraction, α:

$$\frac{\partial \alpha}{\partial t} + \nabla.(\boldsymbol{U}\alpha) + \nabla.[\boldsymbol{U_r}\alpha(1-\alpha)] = 0 \quad (9)$$

$$\boldsymbol{U_r} = \boldsymbol{U_1} - \boldsymbol{U_2} \quad (10)$$

To find the phase fraction in a cell, the equation must be integrated but as this is currently implicit in α, it is a tricky process. To achieve this, an iterative approach is required and this is where the concept of MULES is to be utilised.

3.3. MULES

MULES (Multidimensional Universal Limiter of Explicit Solutions) is a solving technique based on FCT (Flux Corrected Transport). The process involved in MULES is explained in full in the 2013 paper from Santiago Márquez Damián [13] but a brief summary is provided below.

Firstly, the mass conservation equation for the primary phase must be solved, the mass face flux assembled and through this, the new mixture density can be found through a use of `nAlphaSubCycles`. Following this, the compressive velocity at the interfaces must be calculated (as a flux) before the discretised form of the equation for dispersed phase is solved iteratively by the MULES integrator. Once this is done, the updated density (it is an iterative procedure) can be found and this enables the solving of the momentum predictor.

The final step of the procedure requires the use of the PISO (Pressure Implicit with Splitting of Operators) loop. In this PISO loop, the face flux is found and finalised, the pressure equation is assembled, the proposed flux is adjusted dependent on the effect of pressure and lastly, the static pressure equation is reassembled (from p_{rgh} to p).

3.4. porousDriftFluxFoam

`porousDriftFluxFoam` is a modified version of `driftFluxFoam` in OpenFOAM. `driftFluxFoam` is a “solver for 2 incompressible fluids using the mixture approach with the drift-flux approximation for relative motion of the phases” [14]. Russell, the other member of the simulation team covered the mathematical aspect of the Drift Flux equations [15]. The basis of the process aims to solve the mixture continuity equation and the mixture momentum equation.

`driftFluxFoam` (and hence `porousDriftFluxFoam`) can have a variety of viscosity models, settling models and turbulence models implemented into the solution. In the case of this project, the turbulence model aspect was not considered as laminar flow was used.

4. Methodology

4.1. Armfield Rectangular Tank

The main simulation which was to be performed in order to meet the project requirements was a multiphase model of the Armfield Rectangular Tank. An example of this tank was situated in the workshop in the Harrison Building at the University of Exeter. Experiments were carried out on the tank by other members of the team and the simulations set up in this section are intended to replicate and validate the experiments.

This model started out with a meshing process before moving on to setting up the boundary conditions and other simulation parameters (including simulation runtime and solver). The case initially contained 3 directories: *0*, *constant* and *system* (as is standard in an OpenFOAM simulation). The process and contents of each directory for the case are discussed in detail in this section.

4.1.1. Meshing

The first step of the process was the creation of a mesh. This task was completed by the meshing team and details of this can be found in Scobell's report [16]. The outline of the process was to measure the geometry of the Armfield rectangular tank in the workshop and convert this into a 3-dimensional drawing using SOLIDWORKS. The mesh was then created manually using software called Pointwise using an stl (stereo lithography) file.

Once Scobell's Pointwise mesh had been created, the mesh was analysed by OpenFOAM using the `checkMesh` command. The mesh passed OpenFOAM's criteria and an image of the 670,000 cell mesh is shown in figure 2 below.

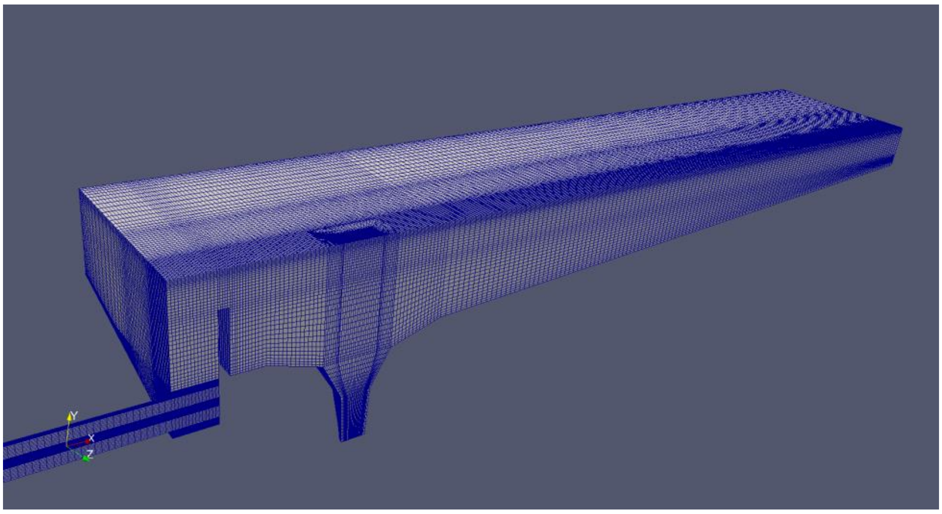

Figure 2: Rectangular Tank Pointwise Mesh

4.1.2. 0 directory

The first directory to consider is that of the *0* timestep directory. This directory represents the beginning of the simulation and contains the initial conditions for the flow. Typically, solvers take the values from the *0* timestep directory and write values into new timestep directories as they're calculated.

In this case, the *0* timestep directory contains 3 files: 'alpha.sludge', 'p_rgh' and 'U' which respectively represent the proportion of sludge in each cell, pressure and velocity. Each file is very similar: it begins with the OpenFOAM banner which defines the name of the object (e.g. "U"). Next it defines the dimensions of the object, followed by the `internalField` and finally the `boundaryField`.

The dimensions are given by the exponent of each SI unit which in OpenFOAM should be defined in the following order: mass, length, time, temperature, quantity, current and finally, luminous intensity [4].

$$[kg\ m\ s\ K\ mol\ A\ cd]$$

For the U file, this is as follows:

```
dimensions       [0 1 -1 0 0 0 0];
```

The `internalField` defines the initial conditions for all of the internal parts of the mesh. For each file in this case, this is just to define the internal field as 0 because the fluid in the tank is to begin at rest. For the velocity, this is done with the following line of code:

```
internalField   uniform (0 0 0);
```

In the case of a scalar (rather than velocity which is a vector), only a single 0 is provided. The `boundaryField` section defines the initial conditions at boundaries. This includes the external wall, the underflow, the overflow, the inlet and the outlet. There are also definitions for the atmosphere (the top, roofless surface) and the symmetry plane (the tank was halved to reduce computational time). These are defined as 0 excluding the velocity at the inlet and underflow (respectively 0.316m/s in the x direction and -0.022m/s in the y direction) and the alpha value at the inlet (0.0002). For example, some of the `boundaryField` for U is shown below:

```
boundaryField
{
    atmosphere
    {
        type                slip;
    }
    inlet
    {
        type                fixedValue;
        value               uniform (0.316 0 0);
    }
}
```

4.1.3. *constant directory*

The *constant* directory contains information relating to the model for the simulation. It will generally include necessary constants which define the substances involved and other global parameters such as gravity. In addition to this, the constant directory contains the `polyMesh` subdirectory which itself contains the mesh files. In this case (as discussed in 4.1.1), the mesh files have already been provided.

The gravity file (defined as ‘g’), defines the direction and strength of gravity, as well as the units. Gravity would subsequently be called by other scripts during the simulation.

Another file in the constant directory is that of `transportProperties`. This file defines the properties of the two phases, the viscosity model and the velocity model. The phases and viscosity model are defined as follows:

```
phases (sludge water);

sludge
{
    transportModel  slurry;

    rho         1438;
}

water
{
    transportModel  Newtonian;

    nu              1.0e-06;
    rho             1000;
}
```

The two phases are sludge and water with their densities given by rho (measured in kgm^{-3}). For water, the viscosity is given by nu but for sludge, viscosity is defined by `transportModel`. For this, the viscosity model ‘slurry’ is used and more details of this can be seen in Mendoza’s report [17].

The velocity model is defined by:

```
relativeVelocityModel general;

"(simple|general)Coeffs"
{
    V0              (0 -0.0038 0);
    a               719;
```

```
    a1              21570;
    //residualAlpha   0.0000123;
    residualAlpha   residualAlpha [0 0 0 0 0 0 0] 0.0000123;
}
```

This gives the parameters involved in settling, including the settling velocity, v0. Further details of the mathematics behind this, including the calculation of the values, can be found in Wye's report [4].

In this project, there were four defined models for the settling parameters, two of which are covered for the rectangular tank and a third for the settling tubes. These are summarised by the table below.

Table 1:Settling Models

Model	Representation	alphaResidual	v_0/ms^{-1}	a	a_1
Model 1	Secondary Sludge	2.086E-08	0.00824	719	7190
Model 2	Half OSP, Half Sludge	1.283E-05	0.0038	719	7190
Model 3	OSP from Batch Testing	1.283E-05	0.00109	1064	10814

The final file in the directory is `turbulenceProperties`. This file is used to define the turbulence in the model. In this case, it is laminar and is hence defined as such:

```
simulationType  laminar;
```

OpenFOAM recognises laminar as a standard option for `simulationType` and therefore does not account for turbulence in the model.

4.1.4. system directory

The *system* directory contains several files including three key dictionary files which dictate the running of the simulation: *controlDict*, *fvSchemes* and *fvSolutions*. In *fvSchemes*, "the finite volume discretisation schemes are defined" and *fvSolutions* contains "controls related to the mathematical solver, solver algorithms and tolerances" [18]. *controlDict*, however, addresses the overall running of the simulation. It provides a means to adjust the timesteps, control the simulation length and indicate which solver was to be used. In this case, the timestep was 0.5s, writing a new time directory every 50s. The simulation length was 1100s and the solver to be used was `porousDriftFluxFoam` which was discussed in section 3.4.

4.2. Settling Tube

4.2.1. Meshing

The settling tube is a vertical cylinder which is a much simpler geometry than the rectangular tank and as such Pointwise was not necessary. For this case, it was easier to create a *blockMeshDict* and run `blockMesh` rather than import CAD geometries into Pointwise.

The first line of code required in the *blockMeshDict* allowed for the vertex locations to be entered in millimetres as opposed to metres.

```
convertToMeters 0.001;
```

`blockMesh` creates its geometries in a block format with each block consisting of vertices and edges (which can be defined as straight or curved). The first step in creating the `blockMesh` was to split the cylinder into 5 blocks as shown figure 3.

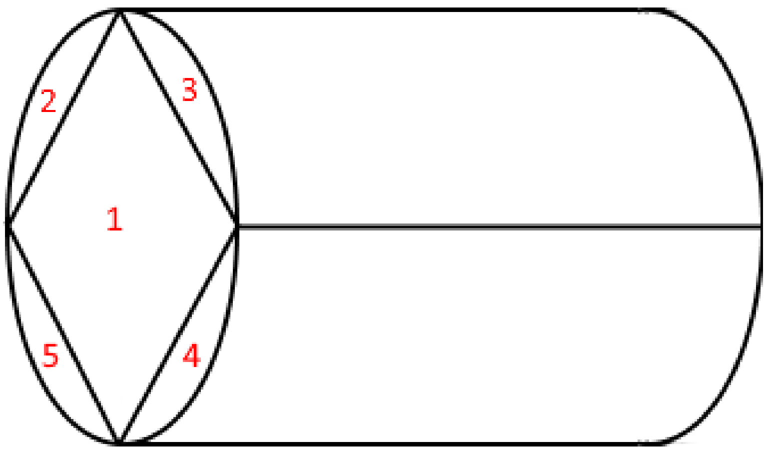

Figure 3: Cylinder Block Formation

The x, y and z coordinates of each vertex was then calculated trigonometrically and defined under ‘vertices’. An example of this is shown below.

```
(0 -25 0)
(-17.68 -17.68 0)
```

```
(-25 0 0)
(-17.68 17.68 0)
(0 25 0)
```

As each of these vertices is defined, they are labelled 0 through 15 and their vertex numbers are used to define blocks later. Before the blocks are defined, some edges had to be defined as arcs (under 'edges') To do this, two of the previously defined vertices were given along with a third point to define the arc. Examples of this can be seen below.

```
arc 0 1 (-9.57 -23.1 0)
arc 1 2 (-23.1 -9.57 0)
arc 2 3 (-23.1 9.57 0)
arc 3 4 (-9.57 23.1 0)
```

Penultimately, the blocks themselves could be defined. The format for defining blocks starts by using hex (for hexahedral block), entering vertex numbers, entering the number of cells in each direction and finally the cell expansion ratios.

```
hex (7 5 3 1 15 13 11 9)
(2 2 100)
simpleGrading (1 1 1)

hex (1 3 2 2 9 11 10 10)
(2 2 100)
simpleGrading (1 1 1)
```

In terms of the number of cells in the mesh, the blocks were temporarily defined as above.

Lastly the 'patches' had to be defined. These are the faces within the mesh. The external walls of the settling tube were defined as 'walls' and the rest were left to be assumed as internal by OpenFOAM. For example, the code for the bottom of the cylinder is shown below.

```
wall bottom
        (
                (9 11 10 10)
                (11 13 12 12)
                (13 15 14 14)
```

```
        (15 9 8 8)
        (15 13 11 9)
    )
```

At this stage, the *blockMeshDict* was complete and so it was inserted into an old tutorial case file to be tested with `simpleFoam`. The mesh was created using the `blockMesh` command and then it could be run with `simpleFoam`. Due to the model just being a static cylinder of water, nothing was observed to happen but it proved that the mesh was created correctly and interacted with OpenFOAM in the expected manner. Figure 4 shows the result of `blockMesh`.

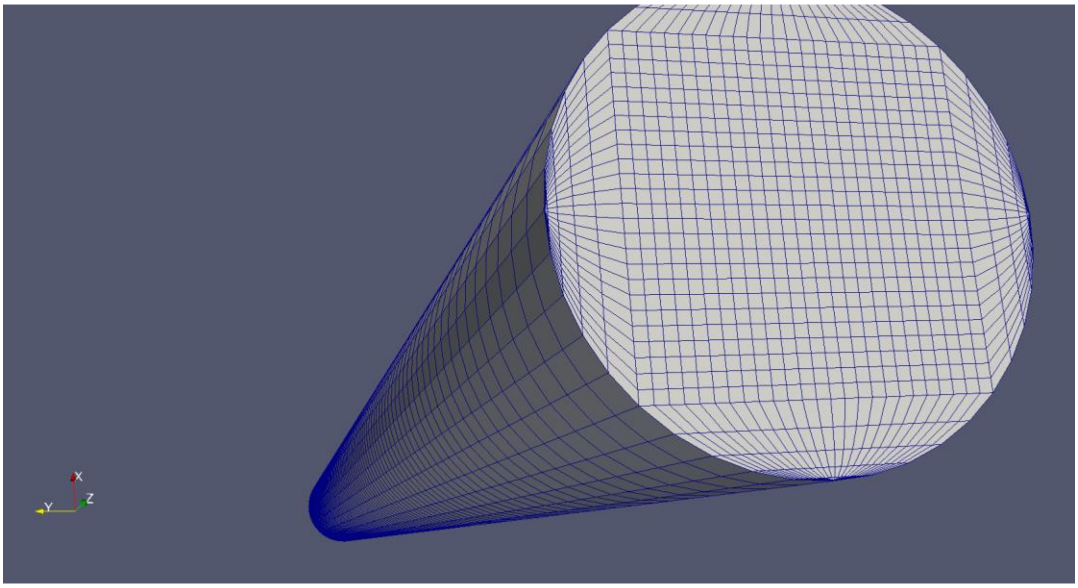

Figure 4: Settling Tube blockMesh

4.2.2. Case Setup

The next step to running the settling tube with `porousDriftFluxFoam` was to alter the rectangular tank case to suit this case. Firstly, the mesh files were removed and replaced with the new cylindrical mesh. The settling tube case was quite different in the sense that it begins with the sludge phase already dispersed in the tank rather than introducing it via the inlet. As such, the entries for underflow, overflow, inlet, etc were removed from the files in the *0* directory and replaced with the correct names for the settling tube. From there, all of the initial conditions could be set to 0 besides the *alpha.sludge* file which needed the `internalField` to be set to different alpha values (the first simulation required an alpha value of 0.00341). This was done with the following code:

```
dimensions      [0 0 0 0 0 0 0];

internalField   uniform 0.00341;

boundaryField
{

    wall
    {
        type            zeroGradient;
    }

    top
    {
        type            slip;
    }

    bottom
    {
        type            zeroGradient;
    }
}
```

Besides needing to alter the runtime (to half an hour or 1800s) and settling model for some cases, there were no other necessary changes for the general setup of the settling tubes.

4.2.3. Mesh Convergence Study

A mesh convergence study was carried out on the previously described case. Eight meshes of different coarseness were devised and each of them was run with `porousDriftFluxFoam` until 600 seconds of simulated time. At this timestep, the highest value of phase fraction was recorded and following all eight simulations, the results could be compared. In order to do this, the maximum recorded phase fraction from the finest mesh was assumed to be the true value and the error between each simulation's value and this value was calculated. The table below summarises the results of the simulations and the subsequent calculations.

Table 2: Mesh Convergence

Number of Cells	Maximum Phase Fraction	Phase Fraction Error
3150	0.00552	0.00568
7200	0.00650	0.00470
14,400	0.00839	0.00281
24,300	0.00886	0.00234
39,270	0.00988	0.00132
57,600	0.0101	0.0011
83,160	0.0109	0.0003
112,500	0.0112	0

For the coarser meshes, the maximum alpha value is seen to be very far from the true value and as the mesh size increases, so does its accuracy. This is seen clearly in the graph of this data in figure 5. A convergence is found where the two finest meshes are accurate to two significant figures of each other and hence the finest mesh of 112,500 cells is sufficient for the simulations.

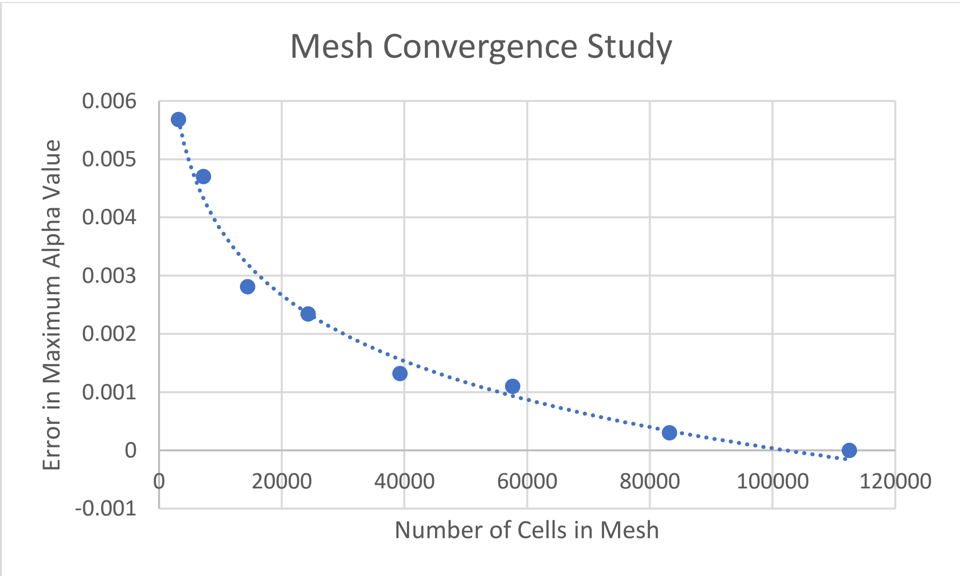

Figure 5: Settling Tube Mesh Convergence

4.3. *Simulations*

To get sufficient data on the different settling models, eight simulations had to take place using the previously defined cases of the rectangular tank and the settling tube. There was a variation in the four settling values (alpha_residual, a, a_1 and V_0) and the proportion of sludge in the model (either at the inlet or across the entire domain). The eight simulations are summarised by the table below.

Table 3: Simulation Summary

Simulation Name	**Geometry**	**Time /s**	**alphaResidual**	**V_0 /ms^{-1}**	**a**	**a_1**	**α**
Model1Armfield	Armfield	1100	2.086e-08	0.00824	719	7190	2e-04
Model2Armfield	Armfield	1100	1.283e-05	0.0038	719	7190	2e-04
Model1_alpha2	Settling Tube	1800	2.086e-08	0.00824	719	7190	3.41e-03
Model1_alpha3	Settling Tube	1800	2.086e-08	0.00824	719	7190	8.08e-04
Model2_alpha2	Settling Tube	1800	1.283e-05	0.0038	719	7190	3.41e-03
Model2_alpha3	Settling Tube	1800	1.283e-05	0.0038	719	7190	8.08e-04
Model3_alpha2	Settling Tube	1800	1.283e-05	0.00109	1064	10814	3.41e-03
Model3_alpha3	Settling Tube	1800	1.283e-05	0.00109	1064	10814	8.08e-04

These simulations were mostly run over multiple cores using the available server space within the College of Engineering, Mathematics and Physical Sciences. There are six available servers, each with 28 cores, for the college. This was done through the use of secure copy, compiling of libraries (the code for `porousDriftFluxFoam` was also included within the cases for server use) and `mpirun`. The following commands allowed the cases to be run on the server (the second and third commands were used in the `porousDriftFluxFoam` directory to compile for the server).

```
Scp -r <file name> <server name>:~/

./Allwmake

./Allclean

decomposePar

mpirun -np 20 porousDriftFluxFoam -parallel > log.porousDFF 2>&1
```

This represents a case run over 20 cores on the server. Once all eight cases had run, the next stage was to use paraview to carry out the post-processing.

5. Presentation of Analytical Results

5.1. Rectangular Tank Results

The collection of results began with the rectangular tank. Paraview could be opened in order to view each timestep from the results. A visualisation of the phase fraction distribution at the final timestep of 1100s is shown respectively for models 1 and 2 in figure 6 and figure 7.

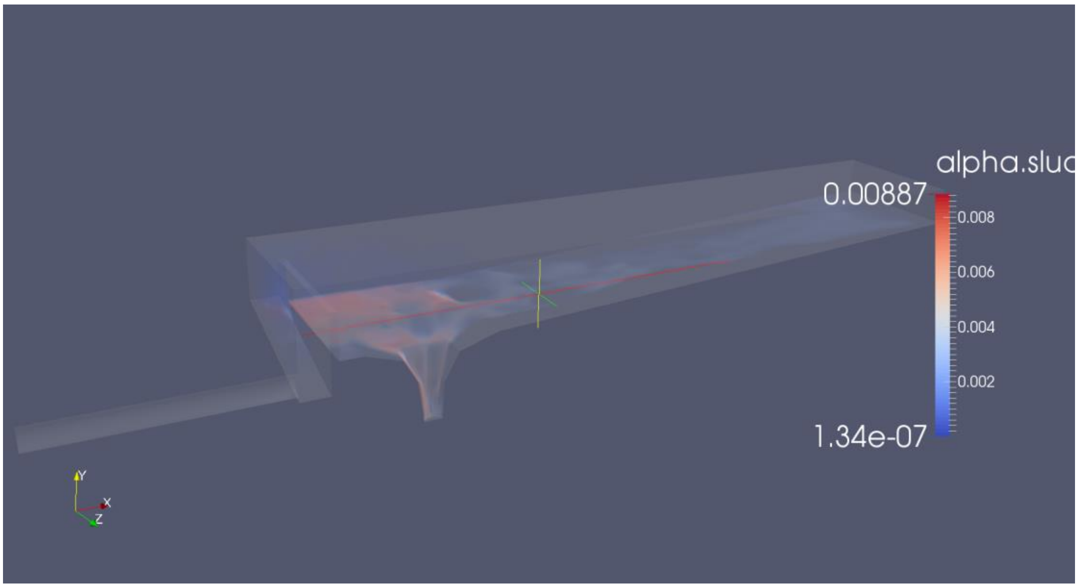

Figure 6: Rectangular Tank Model 1 Phase Fraction

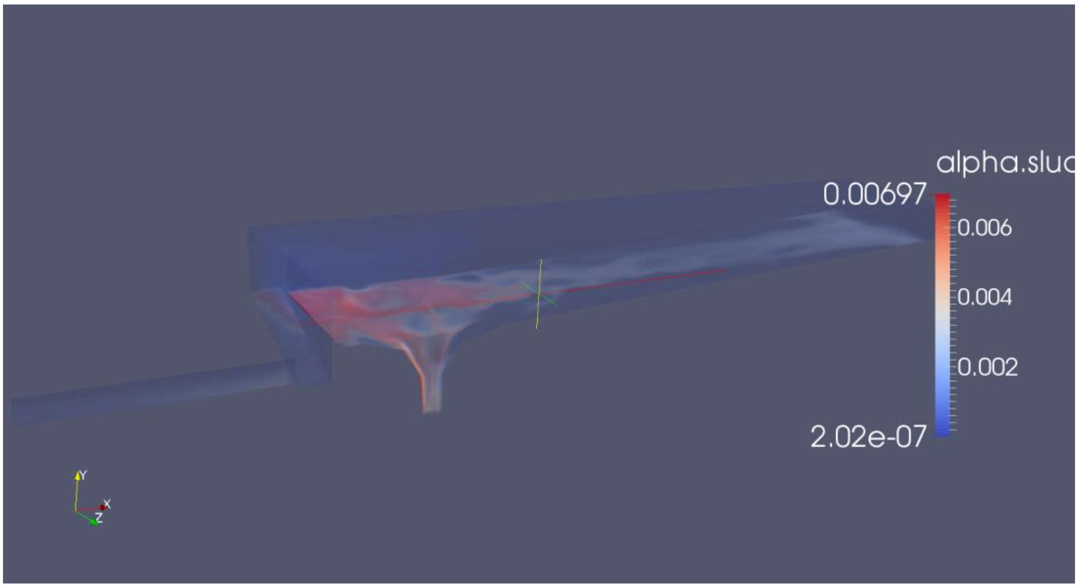

Figure 7: Rectangular Tank Model 2 Phase Fraction

Prior to the running of the simulation, it was hypothesised that more of the sludge (or OSP) would collect up beyond the hopper. However, as figure 6 and figure 7 show, this was not the case: the majority of the sludge almost immediately goes from the weir to the hopper.

The visualisations make it clear as to what would be seen in the rectangular tank but provide very little of numerical interest. In order to create an adequate comparison to the results produced by the experimental team, it was necessary to view the results graphically. Firstly, three points along the length of the tank were selected by the experimental team for their measurements and the three corresponding points in the simulation were looked at with use of the sample utility (a sampleDict was added to the system directory). These points were 20mm, 100mm and 195mm along the length of the tank and these points (and the lines along which measurements were taken) are shown in figure 8.

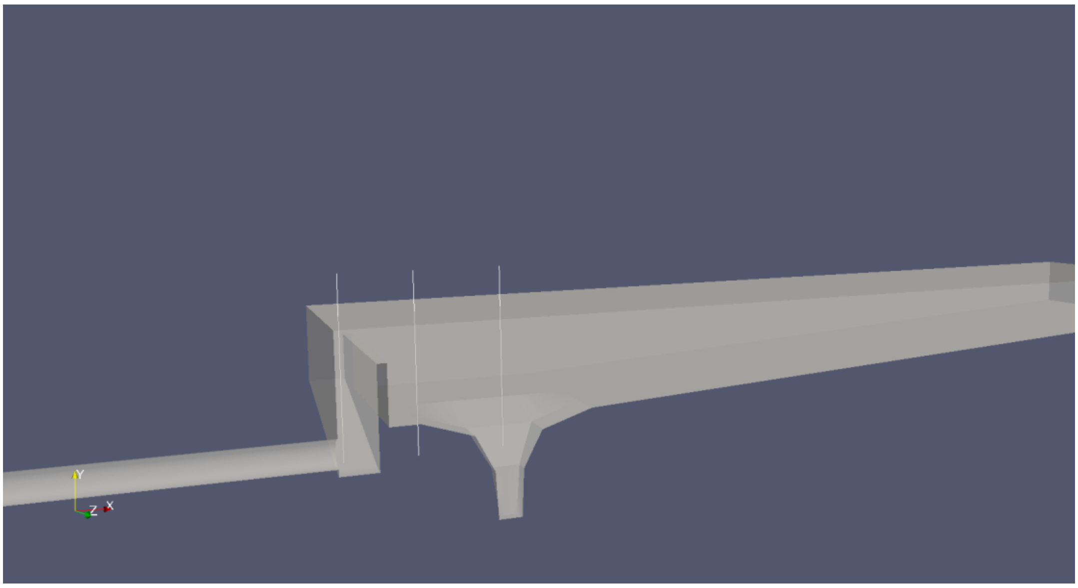

Figure 8: Rectangular Tank Measurement Points

The sample utility then extracted data from the simulation and this could be plotted against the depth. The first plot to look at was the velocity profile at each of the three points for model 1. The plotted graph of velocity against depth can be seen in figure 9.

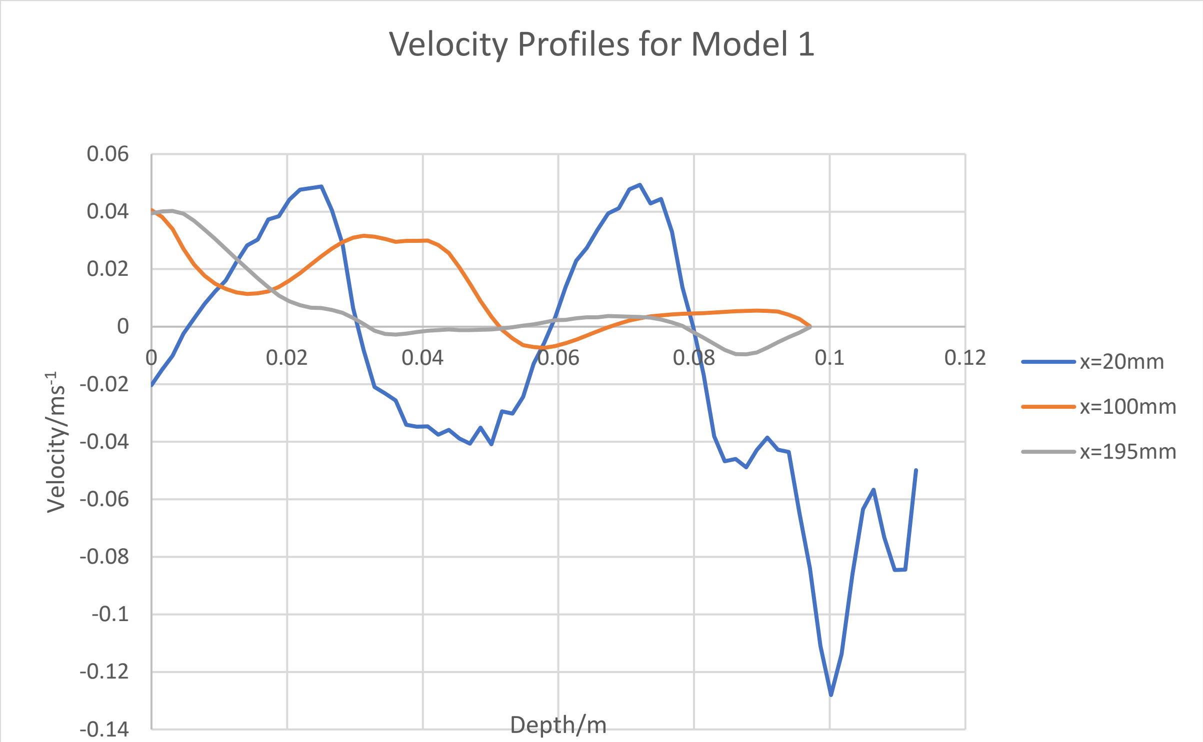

Figure 9: Model 1 Velocity Profiles

This velocity profile shows that the x component of velocity alters drastically as depth changes. It is clear that there is some form of recirculation occurring in the tank: this is indicated by the frequent change from positive to negative velocity. At x=20mm, the velocity in the x direction is generally of higher magnitude and this is due to areas of recirculation forming more further away from the inlet and the weir slowing the flow. The recirculation in the tank can be further confirmed by figure 10 which shows the velocity field within the tank.

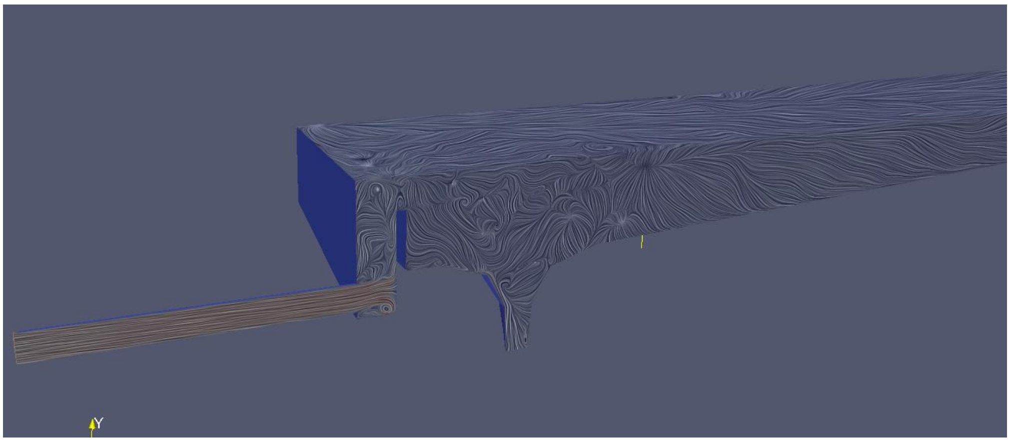

Figure 10: Model 1 Surface LIC

Figure 10 shows a surface LIC filter over the geometry which is a convenient means of observing recirculation regions. Above the hopper, there are a number of vortices which aligns well with the shifting from positive to negative in the velocity profile. To get further information on what is occurring, figure 11 shows the magnitude of velocity in m/s within the tank for model 1.

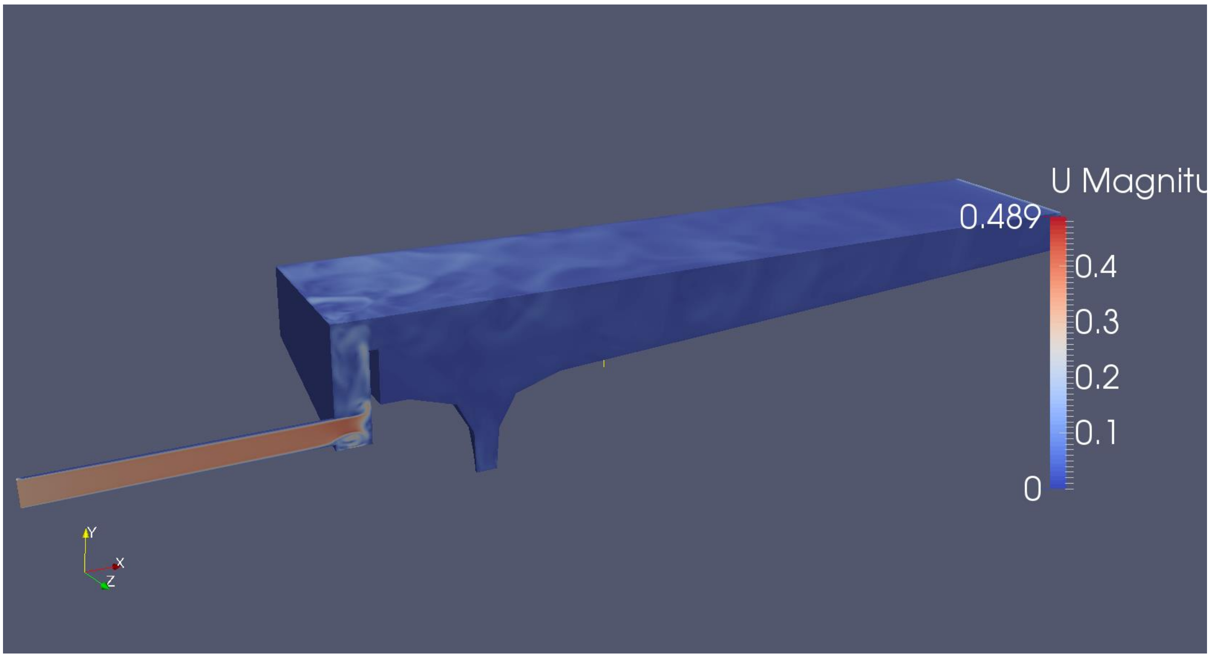

Figure 11: Model 1 Velocity

This figure shows that the fluid in the main section of the tank is relatively static when compared with the inlet pipe. The magnitude of velocity in the main section of the tank is generally less than 25% of the inlet velocity. The velocity is somewhat higher behind the weir and around the surface too. The weir is seen to seriously hinder the flow of the fluid in the tank which ultimately gives more time for the dispersed phase to settle before the fluid passes over the hopper.

It was also necessary to compare models 1 and 2 and as such, figure 12 shows the velocity profiles for model 2.

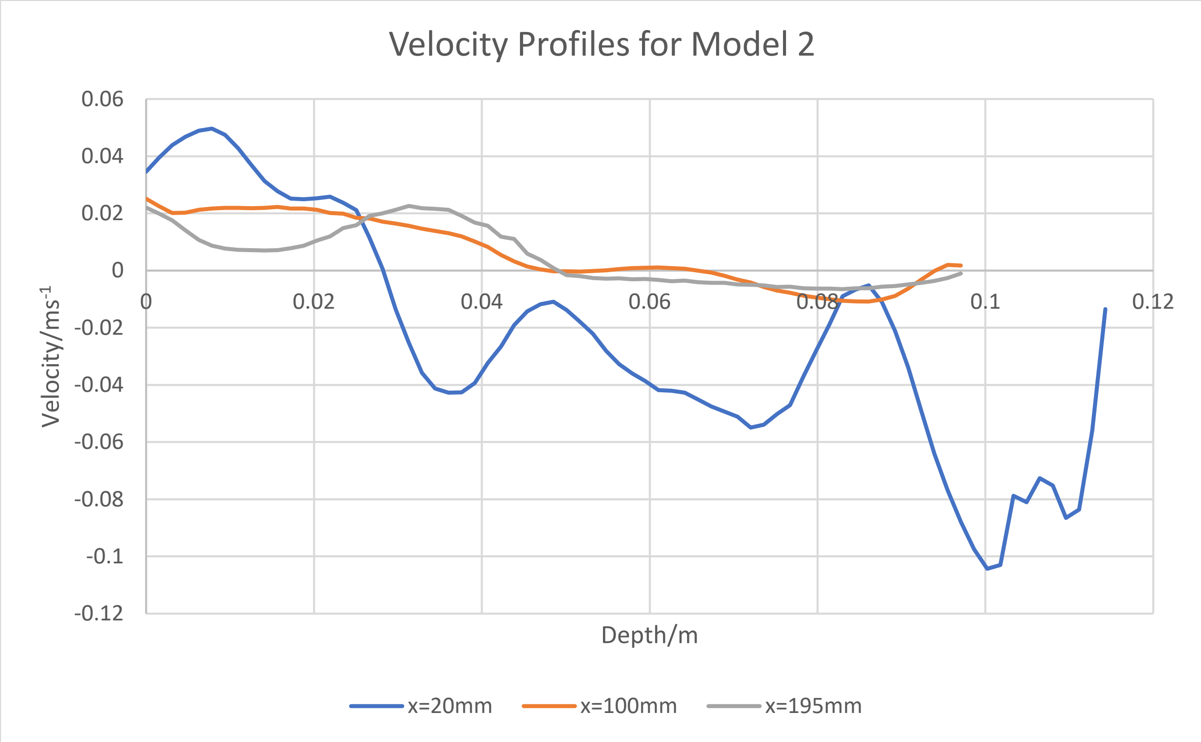

Figure 12: Model 2 Velocity Profiles

In model 2, nearer to the inlet (x=20mm), the shape of the velocity profile differs from model 1. There seems to be less switching between positive and negative: only that it begins with a positive velocity and then becomes a negative velocity at a depth of approximately 280mm. Further down the tank (x=100mm and x=195mm), the profiles are similar to the previous model although the velocity at the surface for both positions is approximately halved in model 2.

The graphs seen in figure 11 and figure 12 had to be compared with the empirical data provided by the experimental team via the use of a propellermeter. More details of the experiment itself can be seen in Baker's report [19]. The following table shows some of the data collected by the experimental team which could then be compared with the results from the simulations.

Table 4: Experimental Data

X coordinate/mm	Depth/mm	Measured Velocity/ms^{-1}	Simulated Velocity/ms^{-1} (Model 2)
20	10	0.0806	0.0475
100	10	0.0499	0.0219
195	10	0.0571	0.0077
20	40	0.0420	-0.0323
100	40	0.0420	0.0083
195	40	0.0442	0.0157

Considering the velocity at the inlet for the simulations was approximately 60% of the velocity used in the experiments, the velocities for model 2 are relatively close to the observed values. It appears the velocities from the simulations are generally a closer match to the empirical results nearer to the inlet. The difference in values is a combination of this difference in inlet velocity, experimental errors and most importantly, the difference between the used settling model and reality. In the case of model 2 (from figure 12), it is a combination of sludge and OSP and any major differences between the empirical and simulated results would indicate that OSP is not such a good substitute for sludge.

In addition to comparing the velocity, it is also essential to analyse the simulated phase fraction distribution. Figure 13 and figure 14 are graphs which show the phase fraction as depth varies for the same three points as previously for models 1 and 2 respectively. These graphs use the data from the final timestep of 1100s.

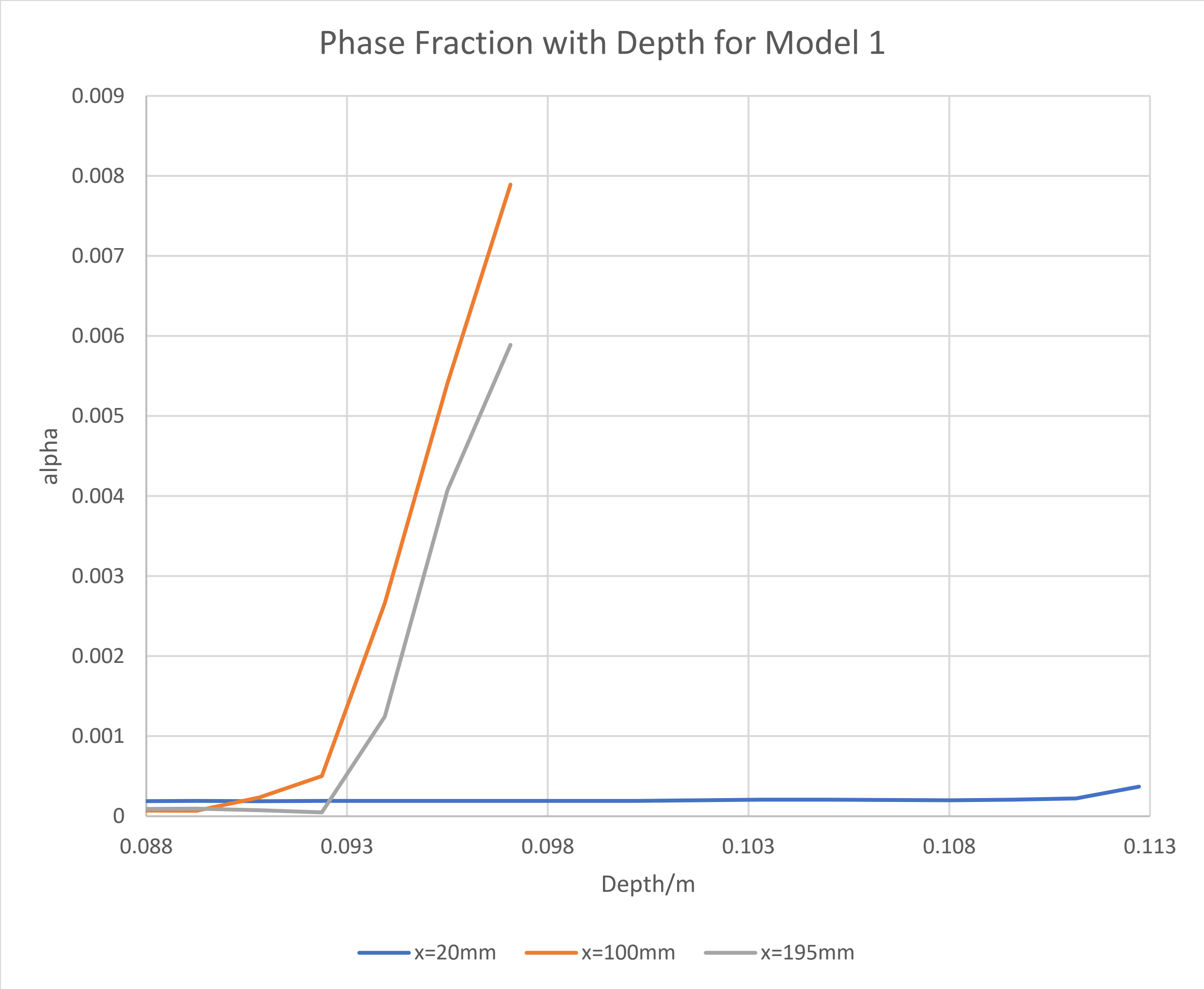

Figure 13: Model 1 Phase Fraction Profile at Final Timestep

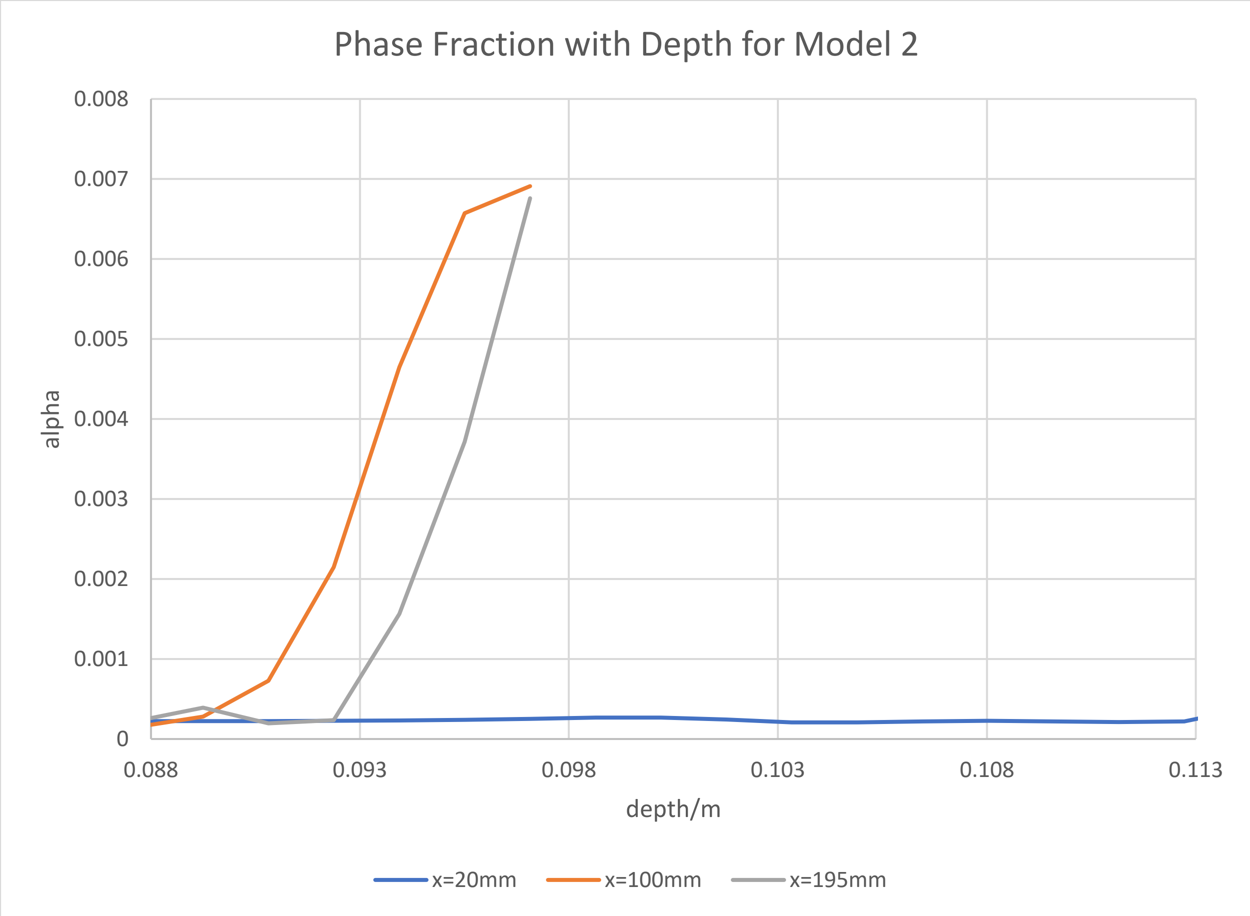

Figure 14: Model 2 Phase Fraction Profile at Final Timestep

As is to be expected, virtually no settling occurs at x=20mm. As a result of this, the phase fraction remains to be around 0.0002. Further up the tank, however, this is not the case. The value of phase fraction rises as depth increases to values between three and four times the size of the phase fraction at the inlet. Model 1 appears to have a higher phase fraction at an x coordinate of 100mm (0.00789 compared with 0.00691) but a lower value at 195mm (0.00589 compared with 0.00676).

Such that the experimental and simulated results for the rectangular tank could be further compared, the figures 15, 16 and 17 were produced by Baker [19]. These three figures respectively show the velocity profiles for 20mm, 100mm and 195mm according to both the simulations and the empirical data.

Generally, the Acoustic Doppler was inaccurate as it did not seem to cope so well with the low velocities. The velocities seen in reality appeared to be much larger than those simulated. This significant difference is again due to the lack of similarity between OSP and sludge when simulated.

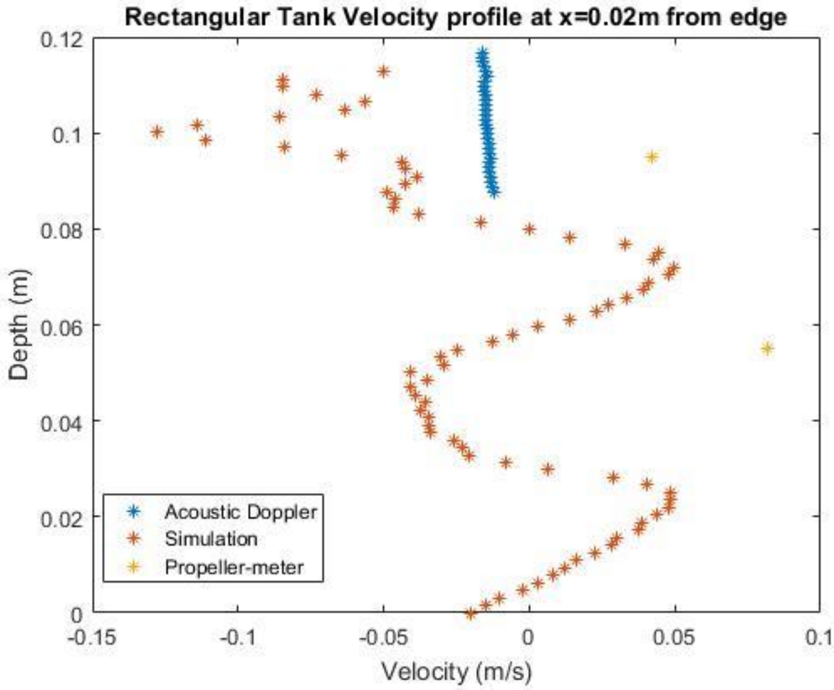

Figure 15: Data Summary for Velocity at 20mm

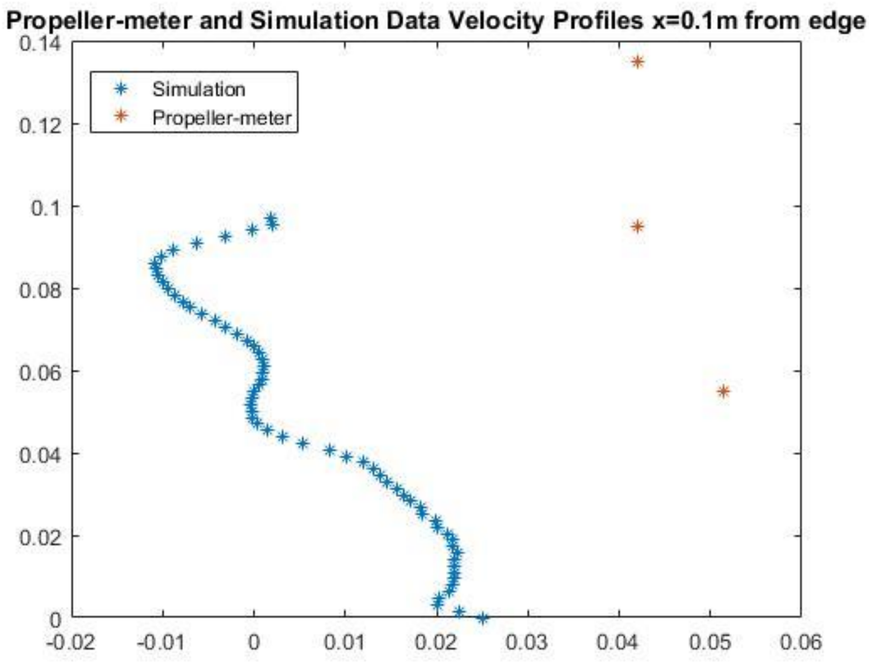

Figure 16: Data Summary for Velocity at 100mm

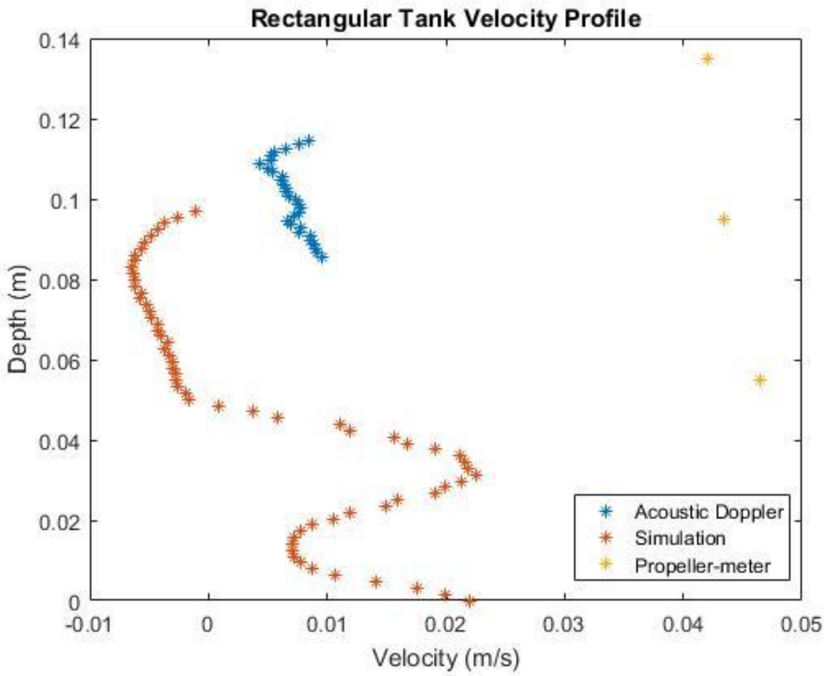

Figure 17: Data Summary for Velocity at 195mm

5.2. Settling Tube Results

The results of the settling tube simulations were necessary to verify that the settling velocity calculation experiments from the experimental team were correctly performed and accurate. The results also allow for a comparison between OSP, sludge and the mixture which could provide or disprove a validation of OSP as a sludge substitute. The results from all six settling tube simulations were collated and two graphs were formed; these graphs are shown in figure 18 and figure 19.

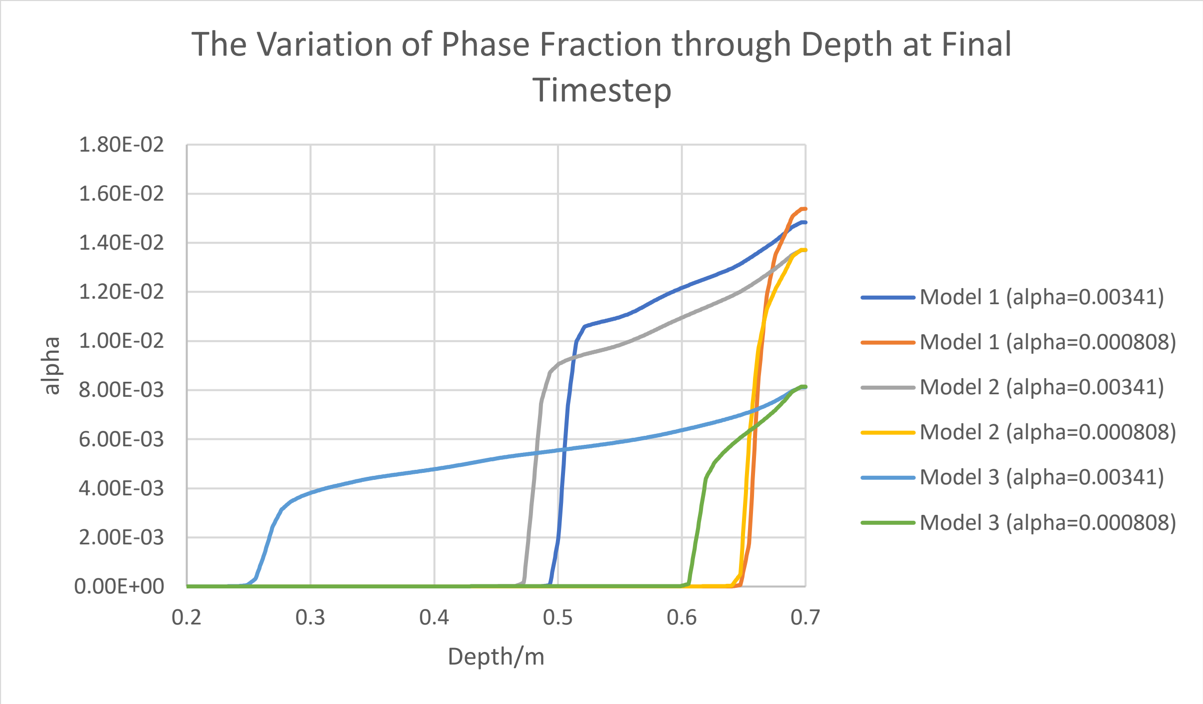

Figure 18: Phase Fraction Profile for Each Settling Tube Simulation

The graph in figure 18 provides a general insight into the final timestep for each model and phase fraction value. As would be expected, the simulations with the smaller initial phase fraction produce a much shorter settled region as the mixtures contain less of the dispersed phase. This can be seen by how the three of them are bunched into the final 10cm of the column. Complementary to this, the higher initial phase fraction produces a settled region within the final 45cm.

Comparing the data for the OSP experimental testing, details of which can be found in Wye's report [4], to the simulation data for model 3 reveals much similarity. For example, the phase fraction value of 0.00341 for model 3 gives a settled region (including the interface) of 44cm. The experimental testing gave a value of 51cm and hence a difference of only 13.7%. This is close enough to indicate that the results of both the experimental and simulation tests for this case are relatively accurate.

By comparing the models, it is evident that model 3 (the OSP) produces a much larger settled region and interface. This suggests that OSP does not behave in a similar manner to sludge as would have been the case if OSP were a good substitute for sludge. Knowing this, the phase fraction profile for model 2 (the mixture of OSP and sludge) would be expected to fall between models 1 and 3 and this is seen to occur for the interface but not the settled region. Additionally, model 2 is significantly closer to model 1 than model 3.

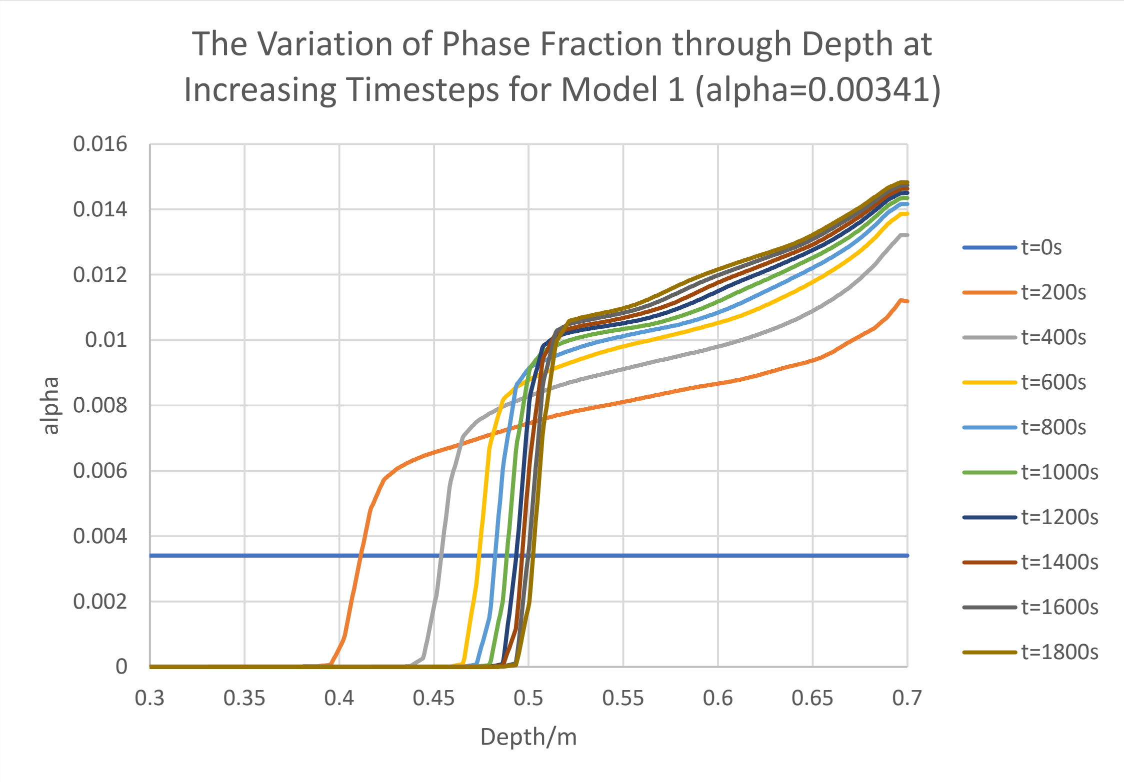

Figure 19: Phase Fraction Profile Through Time

Figure 19 gives a more detailed look at one of the simulations with regards to the elapsing of time. In this case, the higher phase fraction simulation of model 1 (sludge) is observed. The phase fraction profile for each 200s (for the full half hour of simulated time) is plotted on one the one graph and this shows how the column develops over time. It is evident that there is a far greater rate of change in the results between the earlier timesteps than later in the simulation. As the simulation reaches approximately 1200s (20 minutes), the solution has more or less converged to a settled state. After the half hour, there is a settled region (with the phase fraction above 0.0103) of 284mm and an interface of 23 mm. The results from the settling tube simulations certainly emulate the data found by the experimental team, especially in the case of Model 3 (the OSP). The results, however, do show a significant difference in values (despite the general shape of plots being similar) between model 3 and the other two models. This difference in results provides evidence against the effectiveness of OSP as a sludge substitute as it is clear that sludge behaves differently to OSP.

6. Discussion and Conclusions

6.1. Discussion

The purpose of this project as a whole was to validate the use of Olive Stone Powder (OSP) as a viable alternative to sludge in experiments. This aspect of the project produced simulated results for one of Hydro International's recommended sedimentation devices: the rectangular tank. In addition to this, results from settling velocity experiments were also analysed.

As was indicated throughout much of section 5, OSP is not a suitable substitute for sludge as had been theorised. The results of the rectangular tank experiments showed that whilst the general performance of OSP to sludge was similar, the values themselves always seemed to be somewhat different which indicates that it does not behave the same. In the case of the velocity profiles, model 2 (the combination of sludge and OSP) was seen to have generally lower values of velocity. This was seen to be more apparent further down the tank rather than near the inlet. For the phase fraction profile of each model, the shapes of the curves were rather different again. In the case of model 1, the phase fraction values of the two points further down the tank (x=0.1m and 0.195m) were found to be close in value at the surface and then they separate with depth. In total contrast, for model 2, the values were found to begin at the surface with very differing values for phase fraction but gradually drift towards the same value (approximately 0.0068) at the bottom of the tank. Corresponding values for model 3 (OSP) in the rectangular tank can be seen in the report of Russell [15] and provide further evidence that indicates OSP is a poor substitute for sludge.

The difference in values for OSP from sludge was highlighted further in the study of settling tubes. This time, with the inclusion of model 3 (OSP itself), it was more evident. The results from the simulation are shown to be relatively accurate with empirical data but they are still observed to be significantly inaccurate when compared with models 1 and 2. In the case of the final timestep, the space occupied in the column by the dispersed phase for OSP is approximately twice that seen in the other two models. This difference is much too large to be able to adequately validate the use of OSP as a sludge substitute.

This project required much use of the open-source CFD software, OpenFOAM. OpenFOAM, though not quite as user-friendly as some of its commercial package counterparts, held its own in terms of flexibility and reliability. Case files could be fabricated in such a way that any necessary conditions for the case could be fulfilled and the choice of solvers was large. Once generic case files had been created, the directories which defined them could be copied and altered to match the same case with differing values. Due to the multiphase nature of the problem in this project, porousDriftFluxFoam (a modified version of driftFluxFoam) was used as the solver and proved exceptionally versatile. Though the solver typically took a long time to run (even when run in parallel over multiple processing cores), the results produced were as one would expect from a settling case such as this. Additionally, it was the complexity of the multiphase problem that led to high computational demand and as such, long simulation runtimes were anticipated. During this project, paraview was used for the viewing of OpenFOAM results and this package was reliable and efficient when it came to interpret visual results. Producing colourmap representations of the rectangular tank geometry to indicate both velocity and phase fraction fields was both simple to do (provided the cases had been setup and run correctly) and valuable for providing insights of the behaviour of the model. Values for the aforementioned fields could be ascertained and a general representation of the full model could be seen. For example, the phase fraction values of the rectangular tank, when viewed, showed that the majority of the dispersed phase would immediately reach the underflow after passing over the initial weir. Little of the dispersed phase made it further up the tank and hence it was quickly realised that measuring values of phase fraction beyond the underflow was unnecessary.

6.2. Conclusion

This report outlines the process of modelling multiphase flow in a rectangular tank and settling tubes. The method of obtaining the results for these simulations required the use of driftFluxFoam in OpenFOAM. The results were compared with empirical data for Olive Stone Powder (OSP) and the difference in results show that OSP cannot be validated as a substitute for sludge in wastewater experimentation for rectangular tanks. There is potential for further work on this project. This further work includes the testing of different substances for replicating the behaviour of sludge and in addition to this, it would be of interest to see how different solvers or commercial code perform with regards to this problem.

At the beginning of the project, several objectives for this aspect of the work to be completed were defined. The first two objectives were completed via a review of literature as an understanding of multiphase flow techniques were studied and understood. This included a study of MULES. The next three objectives were completed by forming a mesh for the settling tube and performing porousDriftFluxFoam on the two cases to produce the simulations outlined in section 4. Finally, the results from the simulations were reviewed which provided an insight into the flow regime in the rectangular tank and the settling behaviour for the settling tubes. The results also showed that OSP was not to be used as a sludge substitute.

7. Project Management

7.1. Project Management

This report is an explanation of one aspect of the whole project. The full project was the amalgamation of work from seven individuals, split down into three subsections. The three subsections of the project were the experimental team, the meshing team and the simulation team. Naturally, this report makes up part of the simulation team whereas the report of Russell [15] covers aspects of the project pertaining to the simulation of the second sedimentation device, the Swirl-Flo. Early in the formation of the project, each team member was assigned roles based on their respective strengths, in order to give strong functionality of the team as a whole.

Right from the beginning, high standards of organisation and time management were agreed upon as a necessity for the effective running of the project. As such, a Sharepoint folder was created in which all work could be shared between team members and this allowed for convenient accessibility of all that had been done. As well as this, the group deliverables were agreed upon and approximate deadlines for these were put into place. In order to achieve these deliverables on time, a group Gantt chart was produced with smaller required tasks for the deliverables emphasised; this gave an overall view of the dependencies within the project and hence how the team should function to complete the project.

Another essential consideration within the smooth running of the project was effective communication. So that team members were aware of the current status of the project, biweekly meetings were called. There was one informal meeting to discuss the general progress of each team member and to decide on subsequent actions. This meeting included writing up the agenda for the formal meeting later in the week. The formal meeting took place every Friday morning with (ideally) all 7 team members, the project supervisor (Prof. Gavin Tabor) and the client (Dr Shenan Grossberg). This meeting gave the team an opportunity to seek advice for matters regarding the project and enabled the team to plan ahead for the general development of the project. Each of the formal meetings had an assigned team member chairing the meeting and another as secretary to record minutes on all matters arising in the meeting which were to be uploaded to the Sharepoint. To further aid effective communication, the team utilised emailing and online group messaging to enable overall project awareness and required actions for each of the team members.

As is often to be expected in projects, there were a number of technical difficulties. In particular, this occurred with use of OpenFOAM at the university. Though OpenFOAM itself was a reliable code for performing CFD, the servers on which OpenFOAM operated were not. There were multiple occasions whereby the servers did not operate as expected and hence slowed the running of the project. To some extent, these difficulties were mitigated through team members being proactive with time management and setting up and running simulations as early as possible. A potential technical difficulty which was considered from the beginning of the project was that of losing files. The data collected from simulations would always take a large amount of time to produce and as such, the loss of any of this data would seriously impact the smooth running of the project. With this in mind, data was always backed up to external hard drives and in some cases, the Sharepoint.

Specific to this subsection of the project and this report, appropriate management of time was the most important contribution towards project management for the duration. On the whole, unnecessary simulations were avoided and those that were necessary were run as early as possible in order to leave time to analyse the results and hence produce some form of outcome for the project.

Overall, this project was undertaken with great regard to efficiency and effective teamwork. As such, the experience and outcome of the project was generally a success.

7.2. Sustainability

The simulation side of the project, being entirely computational had little regard for sustainability. However, sustainability was a consideration of the group as a whole, especially with respect to the water use on the experimental side. From the beginning of the project the team looked into how much water was necessary for the project and how much water usage was allowed. The team subsequently took these factors into decisions so that the sustainability of the project was met to an appropriate degree.

8. Contribution to Group Functioning

The work from this report aided the general group effort by providing simulations of one of the sedimentation devices (from a mesh provided by the meshing team) and also gave a validation of the settling velocity data provided by the experimental team. A number of multiphase simulations were set up and run using the driftFluxFoam solver to provide details of the flow and settling behaviour in the rectangular tank which could be used to provide evidence for the team against the use of OSP as a sludge substitute.

This report relied on the work of other members of the team and also provided content for the team. For example, the settling tube data was initially provided by Wye [4] and after the simulations had been performed, data was provided to validate the work in that aspect of the project. The data from the rectangular simulations relied on the mesh from Scobell [16] and was necessary for the overall validation studied by Baker [19]. There was also much communication with Russell [15] for work regarding the simulations. Communication between the whole team immensely helped the overall functioning of the team.

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