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# DYNAMIC FLOW MODELLING IN PRECIPITATOR VESSELS - A COMPARATIVE STUDY OF TURBULENCE MODELLING APPROACHES

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## ABSTRACT

Precipitation is a fundamental unit process within the Bayer circuit for the production of smelter-grade alumina, with the predominant technology used in this unit process being the mechanically-agitated draft-tube precipitator. Previous physical modelling studies have identified dynamic behaviour in these vessels which could potentially impact fluid residence time and the ability to obtain adequate solids suspension. In the current study the commercial CFD code ANSYS CFX14 is used to simulate the dynamic, single phase flow behaviour in a laboratory-scale replica of a full-scale precipitator. Simulations are conducted to investigate the impact of mesh refinement and turbulence model selection, with two-equation, Reynolds Stress and the Scale Adaptive Simulation (SST-SAS) models being investigated. The impact of the different modelling choices on the accuracy of the simulations is assessed through comparison of the CFD results with high-quality Laser Doppler Velocimetry (LDV) data obtained in the laboratory-scale vessel.

## INTRODUCTION

Precipitation vessels are critical to the Bayer process for the production of smelter-grade alumina as they are used to crystallise aluminium trihydroxide from solution. Typically the vessels have a height to diameter ratio close to 2:1 and the flow is circulated using an axial flow impeller located in the top of a draft tube which pumps downwards. The draft tube is used to achieve top to bottom recirculation of the fluid in an energy efficient manner. The vessels generally have straightening vanes downstream of the impeller to condition the flow, and a series of narrow slots in the draft tube wall which aid resuspension of the solids if suspension is lost at any time due to mechanical or electrical failure. The geometry of a laboratory-scale replica of a full-scale precipitator is shown in Figure 1.

An understanding of the flow behaviour in these vessels is important as adequate solids suspension and residence time is critical to achieving adequate yield. The shear regimes experienced by solids can influence crystal agglomeration and growth and small improvements in energy efficiency would lead to large economic benefits given the large number of vessels required in a typical alumina refinery.

There is a significant literature on the use of CFD methods applied to the simulation of vessels stirred via a mechanically-driven impeller, covering a wide variety of applications, fluids, vessel geometries and agitator types. However, a review of the literature shows that there is still significant uncertainty regarding the best turbulence models to use for a given application, be it single phase or involving the suspension of particles. The literature is also less complete when it comes to large aspect ratio vessels containing a draft tube.

Lane (2006) has studied the flow in a draft tube precipitator using both the k-ε model and Large Eddy Simulation (LES). He compared the flow in two precipitators that differed only in their height. In order to simplify the modelling he used ¼ of the vessel and applied inlet and outlet boundary conditions at the bottom and top of the draft tube, respectively. The k-ε model results were steady and showed a recirculation zone in the outer annulus of the vessel that was of a similar vertical extent in both vessels. Lane noted that the turbulence intensity was extremely high, so he ran a simulation using LES and observed that the recirculating flow was indeed unsteady. He used these results to explain the observation that the clear layer in the shorter precipitator contained more solids than the exit at the overflow in an operating precipitator.

Derksen et al. (2007) used LES to study the flow in a mixer vessel generated by a Rushton turbine located at the bottom of a draft tube. The instantaneous flow field was found to be highly chaotic, but the mean flow showed a recirculation zone in the outer annulus. They noted the potentially important implication of this flow behaviour in producing short-circuiting and back-mixing in industrial crystallisers.

More recently, Singh et al. (2011) have performed a detailed study of the applicability of various turbulence models to the simulation of single phase flow in a tank stirred by a Rushton turbine. They used ANSYS CFX and tested the standard k-ε model, the Shear Stress Transport (SST) model (with and without curvature correction), the SSG Reynolds stress model (SSG-RSM) and the Scale Adaptive Simulation (SST-SAS) approach. All models predicted the mean axial and tangential flow fields reasonably well. When looking at the turbulent kinetic energy and trailing vortices from the blades it was found that the SST-SAS model performed best although at least 20 revolutions of the impeller needed to be simulated to get good statistics. Overall the SST model with curvature correction performed best on an accuracy versus computational cost basis, although the predicted trailing vortices were too short. On the same basis the worst performing model was the SSG-RSM as it was computationally expensive and did not predict the periodic and random turbulence kinetic energy fields well.

 

It is evident from this review that the best choice of turbulence model depends on the specific details of the problem being solved and whether there is a need to capture transient structures in the flow. The review also highlights the potential need to employ some form of scale-resolving simulation (such as LES or SST-SAS) to obtain the best results in more complex unsteady flows.

In the current study a number of different turbulence models are assessed, in conjunction with systematic mesh refinement, for a high aspect ratio vessel containing a draft tube. The impact of the different modelling choices on the accuracy of the simulations is assessed through comparison of the CFD results with high-quality LDV data obtained in a laboratory-scale vessel.

## EXPERIMENTAL STUDY

Experimental data was obtained by CSIRO Minerals in a laboratory-scale (1 m diameter) precipitator in a study commissioned by Alcoa. The laboratory-scale vessel was a replica of a full-scale tank and included an impeller, straightening vanes and slots in the draft tube wall. The tank was set up to recirculate and did not have any inflows or outflows. Water was used as the working fluid.

Laser Doppler Velocimetry (LDV) was used to measure the vertical component of velocity as a function of radius at several vertical positions within the vessel. Data at elevations of 650 mm and 1150 mm from the vessel floor are used for comparison to the CFD results in this study and the measurement positions are shown in Figure 1. The velocity was averaged over a number of measurements to provide an assessment of the time-averaged velocity at each point. Measurements at each point were taken at several impeller speeds and were found to be very similar when normalised by the impeller tip velocity.

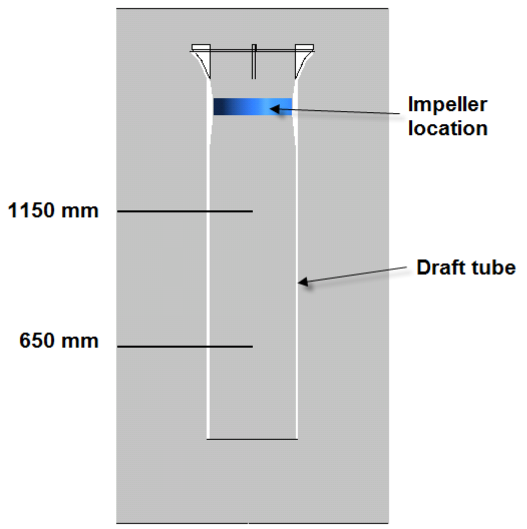


**Figure 1**: Laboratory-scale vessel geometry and LDV measurement positions.

## MODEL DESCRIPTION

### Turbulence Modelling

A number of different turbulence models were tested to determine which could provide a sufficiently accurate prediction at minimal computation cost, an important factor in industrial CFD when complex systems need to be modelled. The flow in the vessel is not governed by flow separation from a curved surface so that the decision was made to use wall functions rather than integrate to the wall. From the experimental data it was known that large-scale unsteadiness needed to be captured.

In preliminary simulations it was found that both the standard k-ε model (Launder and Spalding, 1974) and the Eddy Viscosity Algebraic Reynolds Stress model (EARSM) (Wallin and Johansson, 2000) did not predict any of the velocity field fluctuations expected from the experimental results and so they were discarded and are not reported here. The two-equation SST model (Menter, 1994) and the SSG Reynolds Stress Model (SSG-RSM) (Speziale, Sarkar and Gatski, 1991) were found to give unsteady predictions and were investigated further. Finally, given the unsteady nature of the flow, the Scale Adaptive Simulation (SST-SAS) model was tested.

For transient flows it is known that the standard eddy viscosity models do not predict the turbulence length-scale correctly (Menter and Egorov, 2010), as the equations do not contain sufficient information to do so. The key feature of the SST-SAS model is the use of a transport equation for the turbulence length scale. When the mesh is sufficiently fine, determined from the von Karman length-scale, it switches to an LES-like mode in which the large-scale turbulence structures are resolved. As the mesh is refined, more of the turbulence spectrum is resolved and therefore the turbulence structure of the flow is captured. A key feature of this model is that, unlike LES, the near wall region is modelled using the SST approach so that prohibitively fine meshes are not required to resolve the flow in attached boundary layers at the wall.

### Computational Domain and Mesh

The CFD model was set up to include the full 3-d vessel geometry as the experimental results showed significant asymmetry in the time-dependent flow. The impeller and straightening vanes were not included in the CFD model and instead the impeller was represented using a volumetric momentum source applied in a sub-domain at the same position as the impeller. The momentum source was set so as to achieve the same volumetric flow rate used in the experiments.

An additional simulation showed that a minimum of 1.2 million elements would be required to adequately resolve the detail of the slots in the draft tube wall and that the flow across these slots is only of the order of 5% of the recirculating flow in the vessel. The slots were therefore not included in the current study.

Ten layers of inflation were used on all walls with a 1 mm first layer height and 1.2 expansion ratio. This gave $y^+$ values typically in the range of 20-30. A uniform tetrahedral mesh with edge length of 10 mm was applied in the sub-domain for the momentum source. General guidelines for an appropriate mesh density for the SST-SAS model in this sort of geometry are not available, with the majority of published cases being related to bluff body or aerodynamic flows. Therefore, the edge length of the tetrahedral mesh in the main vessel was systematically reduced and the results assessed. The meshes used are shown in Figure 2.

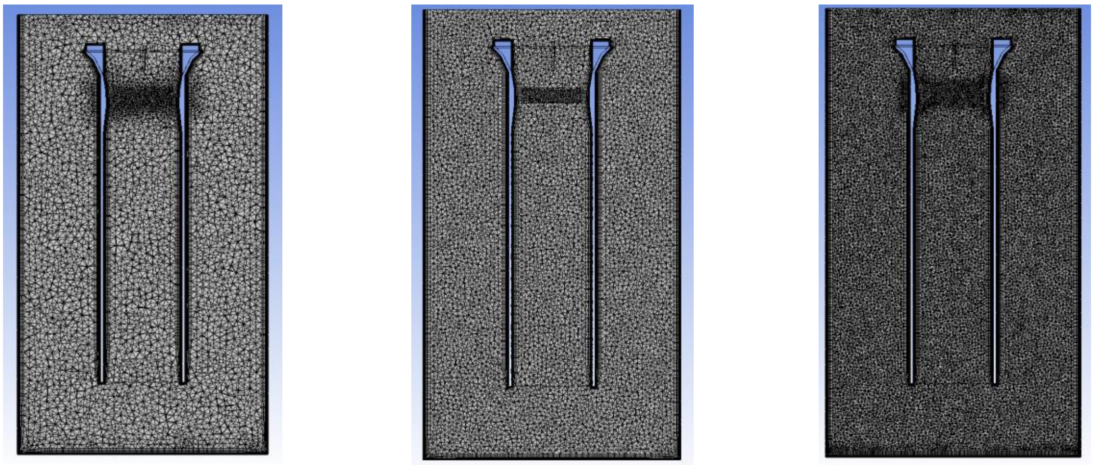

**Figure 2**: The computational mesh used (a) Coarse mesh (840 k elements), (b) Medium mesh (2 million elements), (c) Fine mesh (4.6 million elements)

### Numerical Considerations

The commercial CFD code ANSYS CFX14 was used in the current study. The code uses a vertex-based control volume approach, couples the pressure and velocity via a modified Rhie-Chow procedure and solves the equations using an algebraic multi-grid solver. Second order bounded differencing was used for both the spatial and temporal derivatives.

All simulations were transient and were run for a period of 200 s, which is equivalent to approximately eight residence times in the vessel. The first 50 s of each simulation was discarded and transient averages for flow variables were recorded from this point onwards.

## RESULTS

In Figure 3 the time-averaged CFD predictions and experimental data are compared at positions 650 mm and 1150 mm from the vessel floor. The velocities plotted are the time-average of the vertical velocity component and are normalised by the impeller tip velocity in the experiments.

At the 650 mm position the experimental data shows a very uniform velocity profile inside the draft tube which vindicates the use of a momentum source to represent the impeller in the CFD model. Outside the draft tube the experimental data show a strong upflow at the vessel wall with a downflow next to the draft tube wall, indicating a large recirculating eddy in the lower section of the vessel. At the 1150 mm position the experimental data show an almost uniform, low velocity, upflow in the annulus outside the draft tube, with a slightly higher velocity at the vessel wall than next to the draft tube wall.

Initial simulations were conducted on a coarse mesh with a total of 840,000 elements (Figure 2). This mesh used a 30 mm element size in the bulk of the vessel, which is equivalent to approximately 1/10$^{th}$ of the annulus width. The SST and SSG-RSM models were found to give good convergence using a 0.02 s time step, but the SST-SAS model was found to require a smaller time step of 0.01 s to maintain stability and to achieve a Courant number of approximately 1.0 in the bulk of the vessel, which is consistent with recommendations for this model. With the reduced time step convergence with the SST-SAS model was excellent.

Figure 3 shows that use of the SST model on the coarse mesh provides a good prediction at the 650 mm position. However, the model fails to predict reattachment of the flow to the draft tube wall and hence predictions at the 1150 mm position are poor. It was found that the SST results did not improve with use of the curvature-correction modification.

SSG-RSM is able to predict the key features of the flow on the coarse mesh. However, some details of the flow are not predicted as accurately as others. In particular, at the 650 mm position the model under-predicts the strength of the flow up the outer vessel wall and the strength of the down-flow next to the draft tube. At the 1150 mm position RSM predicts a near-uniform upflow in the annulus, but with a slightly higher velocity near the draft tube. This is opposite to the experimental data which shows a slightly higher velocity on average near the outer vessel wall. A Fast Fourier Transform (FFT) analysis of the fluctuating velocities at a monitor point in the annulus shows that RSM captures only a single dominant frequency (Figure 4).

Analysis of the SST-SAS results on the coarse mesh reveals that the element size is too large to capture the large-scale turbulence structures in the flow. This is highlighted in Figure 4 which shows that only a single dominant frequency is predicted. An iso-surface of the Velocity Invariant Q (calculated as the difference between vorticity squared and strain rate squared) also shows the lack of turbulent structure resolved in the simulation (Figure 5). As a result, the additional term in the SST-SAS model responsible for the LES-like behaviour is zero almost everywhere and the SST-SAS results are very similar to those with the SST model, with poor prediction of the experimental data at the 1150 mm position.

At the next stage of the study the mesh was refined by reducing the element size in the bulk of the vessel to 20 mm to give a “medium” mesh of approximately 2 million elements (Figure 2). The same time step settings used on the coarse mesh were found to also work well on this medium mesh.

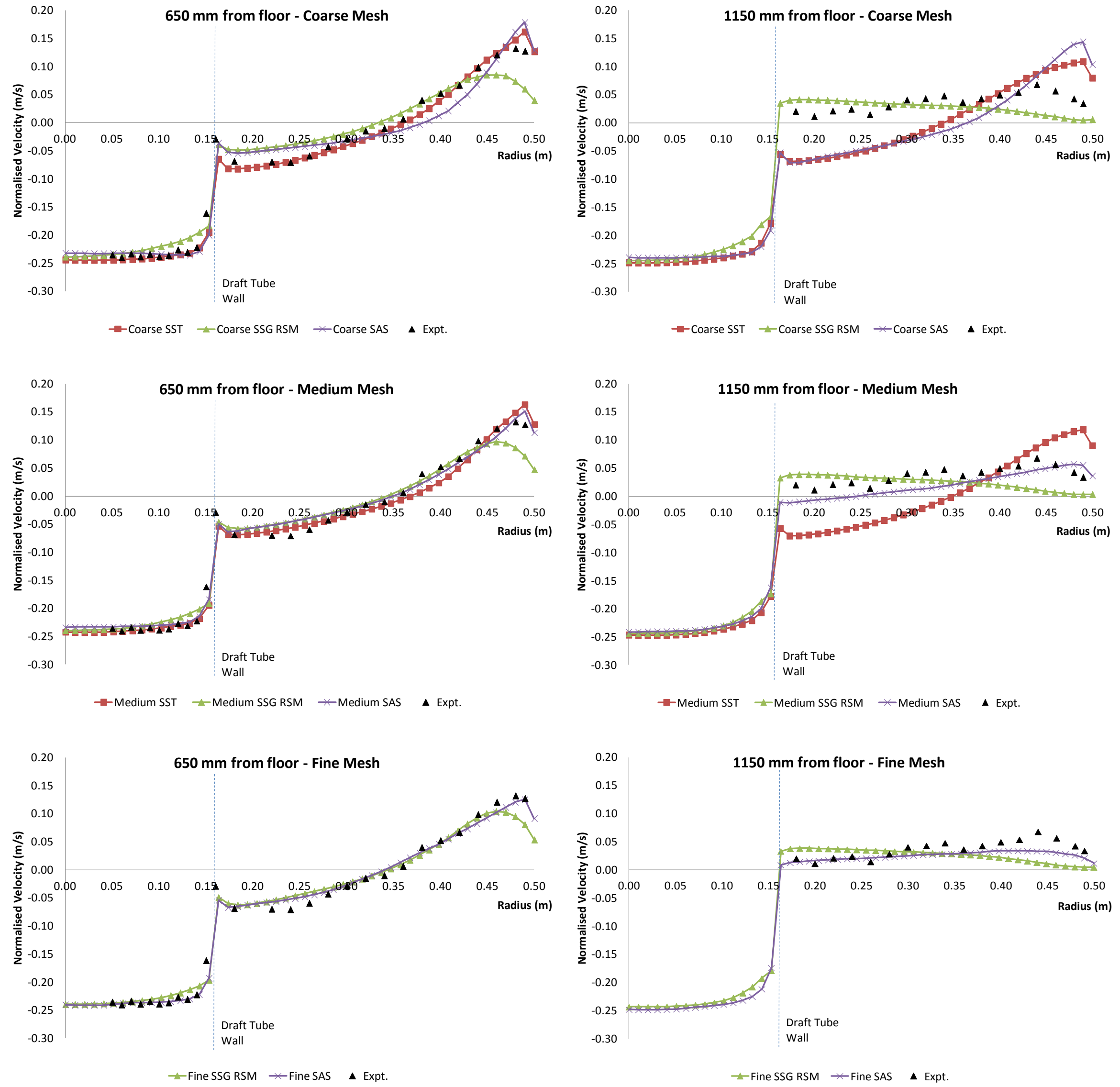


**Figure 3**: Velocity profiles on radial lines 650 mm and 1150 mm from floor of vessel with different mesh densities

Figure 3 shows that the SST predictions did not improve on the medium mesh and hence this model was not investigated further. The RSM shows little mesh sensitivity, although the prediction at the 650 mm position improves slightly. Figure 4 also shows that RSM on the medium mesh predicts the same dominant frequency as on the coarse mesh.

The most significant change on the medium mesh is the improvement in the SST-SAS prediction. Figures 4 and 5 show that the mesh is now fine enough for the SST-SAS model to start to resolve large-scale turbulent structure in the flow. As a result, the time-averaged results show good agreement with the experimental data at both the 650 mm and 1150 mm positions, although at the 1150 mm position SST-SAS predicts a very small down flow next to the draft tube wall which is not seen in the experimental data (Figure 3). Overall, the SST-SAS model gave the most accurate prediction of the tested models on the medium mesh.

A smaller time step was required in the SST-SAS run (compared with the RSM simulation) but the model has the advantage of only solving two turbulence equations rather than the seven in RSM. As a result, the overall solution time with SST-SAS on the medium mesh (5 days on a high-end 8-core server) was only 25% longer than with RSM.

The final fine mesh used an element size in the bulk of the vessel of 15 mm to give a total of approximately 4.6 million elements (Figure 2). RSM shows a further slight improvement in the prediction at the 650 mm position (Figure 3) but is largely insensitive to mesh refinement. Again, Figure 4 shows that RSM on the fine mesh shows no spectral information and predicts the same dominant frequency predicted with the coarse and medium meshes. This is consistent with Figure 5 which shows that even on the fine mesh RSM predicts very little turbulent structure in the flow.

Further mesh refinement allows the SST-SAS model to resolve smaller turbulent structures in the flow as seen in Figure 5. This results in an improvement in the prediction of velocity at the 1150 mm position in particular, but the time-averaged results do not change significantly from those on the medium mesh (Figure 3) and, for the purposes of industrial simulation, the improvement in prediction would need to be weighed against an almost 2× increase in the overall solution time on this mesh.

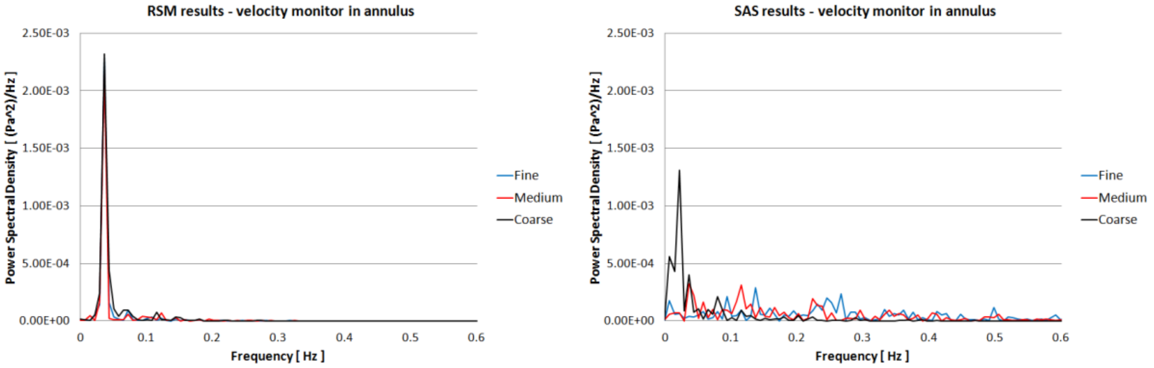


**Figure 4**: FFT analysis of fluctuating velocities at a point in the annulus; RSM runs (left) show a single dominant frequency on all meshes; SST-SAS runs (right) show increased spectral information as the mesh is refined.

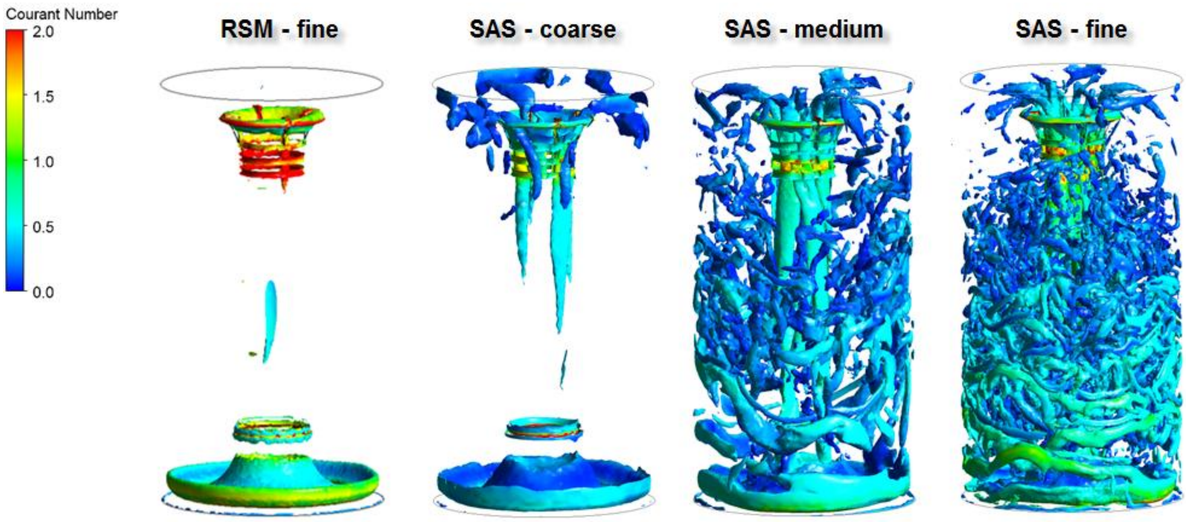


**Figure 5**: Iso-surface of Velocity Invariant Q at 10 $s^{-2}$ showing the lack of turbulent structure resolved with RSM and the increasing structure resolved with SST-SAS as the mesh is refined.

Further analysis of both the RSM and SST-SAS results shows highly anisotropic turbulence in the annulus. This can be seen in Figure 6 which shows statistical Reynolds stresses for the $\overline{uu}$ and $\overline{vv}$ normal stresses from the fine mesh with SST-SAS. This helps to explain why two-equation models, such as SST, are unable to accurately predict the flow in this geometry.

The significant differences between the level of turbulent structure resolved in the fine mesh RSM and SST-SAS predictions is highlighted by looking at vector plots on a plane through the centre of the vessel. Even though the time-averaged predictions appear very similar (Figure 7), the instantaneous velocity fields vary significantly, with the SST-SAS model revealing a far more dynamic flow with a large amount of small-scale structure (Figure 8).

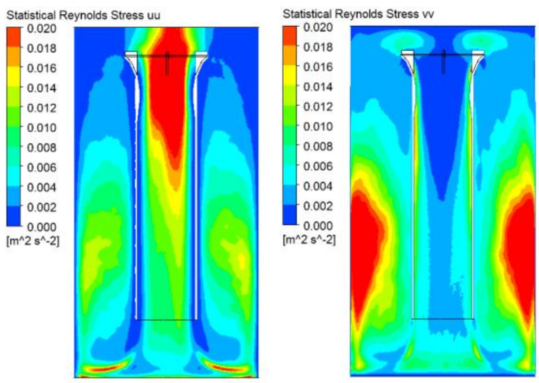


**Figure 6**: Normal stresses from fine mesh result with SST-SAS, highlighting anisotropic turbulence in annulus.

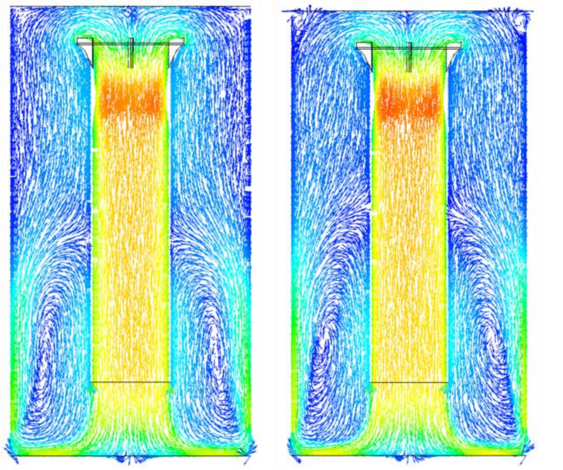

**Figure 7**: Transient average velocities (fine mesh) – SSG-RSM (left) and SST-SAS (right) showing very similar time-averaged behaviour.

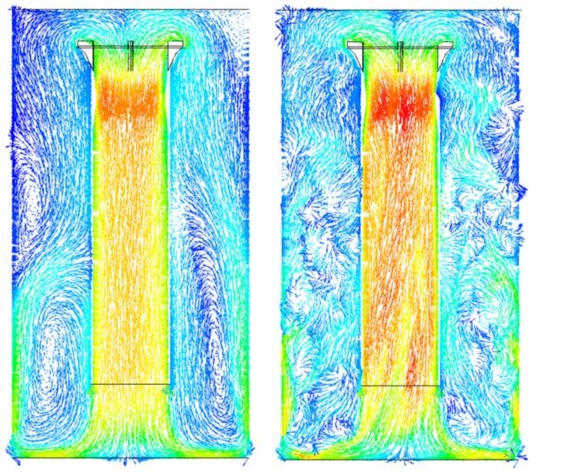

**Figure 8**: Instantaneous velocities (fine mesh) - SSG RSM (left) and SST-SAS (right) showing significant differences in dynamic flow behaviour.

## CONCLUSIONS

From this study a number of conclusions can be drawn about the behaviour of the vessel and the performance of the different models;

1. The flow in the vessel studied is more dynamic and asymmetric than might be expected - this behaviour could affect solids suspension, crystal agglomeration and growth, and particle residence time.
2. Good agreement with the experimental data can be achieved in this type of vessel without the need to explicitly model the impeller – this significantly reduces the model complexity and the mesh size required.
3. Two-equation models perform poorly in this geometry due to the highly anisotropic nature of the flow.
4. The SSG-RSM is able to predict the key features of the flow on a fairly coarse mesh and is fairly insensitive to mesh refinement – this is potentially a good model for initial engineering design given the low computational cost with the coarse mesh.
5. SST-SAS shows the greatest sensitivity to mesh size, which is expected based on the model formulation. There is a need to assess whether the model is resolving sufficient turbulent structure on any given mesh and systematic mesh refinement is likely to be necessary for any new situation. SST-SAS gives the closest match to the experimental data of all the tested models when the mesh is refined.
6. SST-SAS is robust and on a moderate mesh gives good prediction with only a small increase in run time compared with RSM. This confirms that SST-SAS can be practically used for engineering simulations in this type of vessel.

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## REFERENCES

DERKSEN, J.J., KONTOMARIS, K., McLAUGHLIN, J.B. and Van den AKKER, H.E.A., (2007), "Large-eddy simulation of single-phase flow dynamics and mixing in an industrial crystallizer", Chem. Eng. Res Des., **85**(A2), 169-179.

LANE, G., (2006) "Flow instability in an alumina precipitator fitted with a draft tube circulator", Proc. Fifth Int. Conf. on CFD in the Process Industries, 13-15 December.

LAUNDER, B.E. and SPALDING, D.B., (1974), "The numerical computation of turbulent flows", Comp. Meth. Appl. Mech. Eng., **3**, 269-289.

MENTER, F.R., (1994), "Two-equation eddy-viscosity turbulence models for engineering applications", AIAA J., **32**(8), 1598-1605.

MENTER, F.R and EGOROV, Y., (2010), "The Scale-Adaptive Simulation method for unsteady turbulent flow predictions. Part 1: Theory and model description", Flow Turbulence Combust. **85**, 113–138.

SINGH H., FLETCHER, D.F. NIJDAM, J.J., (2011), "An assessment of different turbulence models for predicting flow in a baffled tank stirred with a Rushton turbine", Chem. Eng. Sci., **66**, 5976–5988.

SPEZIALE, C.G., SARKAR, S. and GATSKI, T.B., (1991), "Modelling the pressure-strain correlation of turbulence: an invariant dynamical systems approach", J. Fluid Mech., **277**, 245-272.

WALLIN, S. and JOHANSSON A., (2000), "A complete explicit algebraic Reynolds stress model for incompressible and compressible flows", J. Fluid Mech., **403**, 89-132.