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What is important in the simulation of spray dryer performance and how do current CFD models perform?

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Abstract

Spray dryers are of considerable importance in many industrial drying operations, yet their modelling has been relatively neglected. Here we present a summary of many years work performed at Sydney University investigating the fundamental flow behaviour in dryers and their modelling using a commercial CFD code. The key point to emerge is the need to perform three-dimensional, transient calculations and to include hindered drying and wall interaction models if important issues of flow stability and wall deposition are to be studied. This issue of the need to have proper resolution of the flow at an affordable cost is addressed.

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1. Introduction

Spray dryers are used in a wide and important range of processes associated with food, detergent, minerals, pharmaceutical and other product processing. Despite their importance, the modelling of the physical processes governing the performance of dryers is relatively poorly developed. Recently, Langrish and Fletcher [1] have reviewed the state of CFD modelling of dryers and have noted that, whilst significant progress is now being made, many modellers or industries are not using this information to the full.

The key issue in dryer operation is flow stability, i.e. the need to avoid highly unsteady flows. Such flows can lead to significant wall deposition of partially dried product which sticks to the wall, resulting in a build up of crust. This material can then potentially catch fire due to over-heating in for example milk dryers, leading to significant product loss or material can break loose, causing exit pipes to be blocked and/or product contamination. This results in the need for frequent maintenance shutdowns, resulting in significant costs and production loss.

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In this paper, we present a summary of the work performed at Sydney University to develop an as complete as possible, validated model of spray dryers. We have examined both short form and tall form dryers and have successfully modelled many important aspects of both dryer types.

2. Model description

In this section we break down the important components of the modelling process and present our views as to the current state of modelling capabilities. In this paper all the results presented have been obtained using the CFX4 or CFX5 software packages from ANSYS CFX [2]. Whilst the comments are based on simulations using these specific software tools, they are more generally applicable.

2.1. Modelling approach

To our knowledge virtually all spray dryer modelling is performed using a mixed Eulerian/Lagrangian approach, in which the single phase Reynolds Averaged Navier Stokes (RANS) equations are solved to determine the flowfield. The droplets are modelled using the Lagrangian technique and iterative coupling between the conservation equations for mass, momentum and energy is required because of the high inter-phase transfer rates. This modelling choice immediately presents some computational challenges, since in our experience full-scale industrial dryer simulations require three-dimensional, transient flow simulations. Therefore, the Lagrangian transport model must be transient, which necessitates considerable storage requirements if reasonably large numbers of representative droplets are to be used. For large-scale simulations, there is also the issue of parallelization required to avoid excessive run times, which is usually performed using domain decomposition. In this case, Lagrangian particle tracking can be hard to implement in an efficient manner, as particles will rarely remain in one domain.

2.2. Turbulence modelling

Observations of the flow in a pilot-scale spray dryer by Southwell and Langrish [3] have shown the presence of significant flow instabilities, ranging from large scale drifting of droplets if the inlet flow is not swirled, to regular precession if there is inlet swirl. This immediately sets the requirement for three-dimensional simulations of the complete geometry and the use of time accurate simulation methods. It is important to note, as will be emphasized throughout the paper, that the important phenomenology is transient and three-dimensional in nature. Despite this, many workers continue to perform two-dimensional, steady-state CFD simulations (e.g. [4]) that are of very questionable validity for design purposes.

Extensive modelling work for sudden pipe expansions [5,6] has shown that the gross features of this complex transient flow can be captured using relatively simple models based on the Reynolds Averaged Navier Stokes (RANS) equations. Provided that the computational mesh and timestep were fine enough, it was possible to quantitatively reproduce the dependence of the precession frequency of a jet in a sudden expansion flow as a function of swirl number using the k- ϵ turbulence model [5].

Perhaps the surprising feature of this work is the fact that the standard $k-\varepsilon$ model and log-law boundary conditions were used successfully. It appears that, provided the mesh is fine enough, the important large scale motions get resolved and the $k-\varepsilon$ model acts to model the transport processes at the small scale. This could be thought of as a Very Large Eddy Simulation (VLES), where the $k-\varepsilon$ model is used as the subgrid-scale model and its influence is not removed at larger scales. We therefore expect this approach to be somewhat diffusive and to be restricted in its applicability to prediction of the large scale motions. A recent paper by Wegner et al. [7] provides a direct comparison of transient RANS simulations with LES simulations for a swirl burner. They discuss in detail how if the averaging is considered to be ensemble averaging rather than temporal averaging that this approach is justified but that its accuracy may be limited by the equilibrium assumptions made in the closure. They used a Reynolds stress model, as in their case the $k-\varepsilon$ gave steady solution. Their simulations were for much higher swirl numbers (0.75 compared with 0.1–0.2 in our dryer work) which most likely explains this. They found surprisingly good agreement with the observed processing frequency (as we do) and good agreement with the flow fields but the energy contained in the coherent PVC motion was underpredicted. They also highlighted the importance of accurate numerical methods.

The development of Detached Eddy Simulation (DES) models that explicitly remove the effect of the turbulence model in zones where the important energy carrying eddies are resolved is expected to improve these simulations further [8]. Wall effects, together with the need to couple with droplet flows, are very important in spray dryers and therefore the use of Large Eddy Simulation (LES) is seen as prohibitively expensive for use in full-scale industrial dryer simulations.

2.3. Droplet transport

The droplet behaviour is modelled via the Lagrangian approach which allows the history of many (typically tens of thousands) droplets to be followed. This allows the significant variation of drying histories to be followed and regions of droplet recirculation or wall impingement to be identified. The process of droplet tracking is commonplace in steady-state simulations, where the flow field is converged, droplets are tracked through this flow and then the flowfield is recalculated allowing for the droplet interaction effect. After many such coupling a quasi-steady solution is reached and convergence is achieved. In this approach only the droplet source terms to the continuum equations need to be stored.

However, in the transient case droplets must be tracked for just a single timestep and the positions and state (temperature, velocity, dryness etc.) must be stored. New droplets must be injected at the inlet at each timestep. In addition, it is important to store information regarding the turbulent eddy lifetime and length-scale used in the dispersion model so that the droplet dispersion is properly accounted for in the simulation. This adds a significant additional memory requirement and requires longer simulation times. Whilst in steady simulation droplets are tracked until they either exit the chamber or stop at a wall, in the transient case no droplets reach the exit for a significant period and thus the computational time must be long enough for the droplet tracking to reach a quasi steady-state.

We have investigated the possibility of reducing the cost of these simulations by using an Eulerian flow representation of the droplets, so that they can be modeled as a second phase. This has many potential benefits, including improved parallelization of the solution algorithm and reduced storage. However, we have also identified many disadvantages, including the loss of the time history of individual particles (so that each finite volume would contain particles with an average temperature or average humidity preventing tracking of dry particle that get entrained in wet zones), the difficulty of modelling turbulent dispersion and the inability to model interacting jets. These issues are discussed in detail elsewhere [9,10].

2.4. Droplet drying

Proper modelling of the drying behaviour of the droplets is essential to ensure that the quantitative prediction of the droplet behaviour in the dryer is correct. Nijdam et al. [11] have shown that the Lagrangian approach is reasonably accurate for modeling droplet evaporation. However, droplets in spray dryers contain solids and it is therefore important to allow correctly for hindered drying due to the presence of the solids. Langrish and Kockel [12] have developed a simplified drying model for incorporation into CFD codes, and this has been successfully used by Harvie et al. [13] to simulate milk drying behaviour in a tall form dryer. It is noteworthy that the Lagrangian treatment of droplets fits in well with the need to solve for hindered drying, as individual representative droplets are followed, allowing for detailed heat and mass balances to be performed. However, much work remains to be done in this area to develop detailed models of drying that include spatial variation of moisture content in the droplets that can be incorporated into CFD simulations.

It has traditionally been thought that the amount of drying in most spray dryers is limited by equilibrium between the outlet gas and the dried particles (the "exhaust gas locus" concept [14], and the recent observations of Jindal and Boonyai [15]) for a pilot-scale dryer support this suggestion. However, there is some evidence that the drying performance of small scale (pharmaceutical type) spray dryers is limited by the particle drying kinetics [16]. In terms of the wall deposition process, it is also being recognized [17] that improved drying kinetics models are required to predict the temperatures and moisture contents of powders when they are close to the walls of dryers of any size. The main approaches to predicting the drying kinetics for particles include:

- 1. The characteristic drying curve [12,18].
- 2. A shortcut solution to the diffusion equation [19,20] and other diffusion models [21,22].
- 3. Receding-plane type models [17,23] and others that include both convection and diffusion as transport processes [24].

The consequences of applying these drying kinetic models in spray dryers have not yet been assessed. Hence, much work remains to be done in this area to implement detailed models of drying that include spatial variation of moisture content into CFD simulations.

2.5. Wall deposition

A very important aspect of dryer operability is the accumulation of droplets/particles on the dryer walls or in the exit regions. Using the Lagrangian approach allows the fate of individual representative droplets to be determined when they reach the walls. Their local moisture content and temperature is known, allowing the determination of the expected contact regime, i.e. sticking or bouncing. Ozmen and Langrish [25] have developed a model for milk droplet wall interaction behaviour and related it to the sticky point temperature. In simulations, control of the droplet behaviour at the wall is available by the setting of a coefficient of restitution that depends on the local droplet conditions. This approach has been applied to predict wall deposition for a milk dryer [13].

2.6. Particle agglomeration

Many dryers operate in a regime where particle agglomeration is important and determines the character of the final product. Note that near the nozzle liquid droplets coalesce but near the exit the partially dried solids can agglomerate. Practically, the desired product size and character is determined using empirical or trial and error based knowledge. There are significant challenges in predicting agglomeration due to the need to determine particle proximity and the outcome of droplet/particle interactions. So far, the methods that have been successfully used in, for example, crystallization, floc growth etc. have not been applied in dryers. There is the need to reformulate the well-developed Eulerian models in a Lagrangian framework, which means moving away from the population balance approach to one where representative droplets are considered for agglomeration. A discussion of these issues and example simulations of droplet agglomeration in a spray can be found in Guo et al. [26].

Experimental work has been performed to assist with the validation of such models [27] and we have developed agglomeration models based on both the Eulerian and Lagrangian frameworks. Our assessment is that the Lagrangian framework is much more useful for spray dryer simulations, because of the relative ease of modelling turbulent dispersion and computational efficiency. A detailed comparison of the models and their properties can be found elsewhere [10,11].

3. Simulation results

In this section we present some example results from simulations and use them to illustrate the points raised above. The results are split between simulations of tall and short form dryers, since each has rather different issues to be addressed. In tall form dryers, the flow is much closer to plug flow, and there is much less unconstrained space in which flow instabilities can develop. Thus steady simulations are appropriate in this case. Conversely, in short form dryers flow instabilities can develop easily and are a key feature of the simulations.

3.1. Tall form dryers

Two-phase (air and droplets) simulations have been performed for a co-current tall-form spray dryer belonging to the New Zealand Dairy Research Institute. These simulations were based on experiments conducted by Bloore [28] in a large-scale pilot plant, who was investigating the performance of a 10 m tall Delaval dryer in drying milk. The particular dryer was composed of a 7 m high and 2 m diameter main chamber, below

which was located a 3 m high bustle which tapered down to the outlet pipe located at the centre and base of the vessel. Air heated to approximately 210 $^{\circ}$ C entered the driver through a circular port located at the centre and

vessel. Air heated to approximately 210 $^{\circ}$ C entered the dryer through a circular port located at the centre and top of the main chamber. Two alternative inlet ports were used. These were one small or one large, having internal diameters of 0.20 m and 0.31 m, respectively. Feed was injected into the main chamber through a single downward facing hollow cone nozzle, located just below the inlet port at the top of the main chamber, and concentric with the axis of the dryer. The initial solids concentration of the feed was approximately 50% on a wet mass basis.

Unlike the single phase (air only) counter-current tall-form simulations that were performed previously to this test [29], we were able to perform these simulations using a steady-state assumption. That we were able to employ such an assumption is a result of the relatively simple flow pattern existing within a tall-form co-current dryer, with flow being primarily along the axis of the dryer from top to bottom, with no tendency to produce a transient flow. Milk droplets were simulated in a Lagrangian fashion, with the drying model of Langrish and Kockel [12] used to calculate their mass loss rate, and the model of Hennigs et al. [30] was used to calculate wall restitution effects. Heat transfer between the particulate and gaseous phases was also simulated in a fully coupled manner, with the gas treated as being weakly compressible. Two thousand droplet tracks were used to represent the droplet phase, and the mesh was composed of approximately 340,000 elements. The size distribution of droplets entering the chamber was chosen to model the form of the size distribution of the product particles, as reported experimentally [28]. The CFX4 computational code was used with the QUICK scheme applied to the momentum equations and second order upwind with the Van Leer limiter to the remaining equations.

The most interesting aspect of dryer behaviour highlighted by these simulations is the dependence of droplet trajectories on the relative momentum of the air and feed inlet streams. Frame (a) of Fig. 1 shows 50 sample droplet tracks produced during a large inlet throat simulation, while Frame (b) of the same figure shows the same view produced during a small inlet throat simulation. Note that, as the total gas inlet flowrate is the same



Fig. 1. The trajectories of 50 sample droplet tracks produced using the large and small inlet throat simulations. The initial droplet speed in both cases was specified as $v_{nozzle} = 70 \text{ m/s}$. The colour of each trajectory indicates the time each droplet has spent within the dryer. Note that the time scales have been truncated, since in Case (a) some droplets spend considerably longer than 30 s within the chamber. (For interpretation of the references in colour in this figure legend, the reader is referred to the web version of this article.)

for both tests, the momentum of the gas inlet stream in the small throat case is over twice as large as that in the large throat case. The results show that with the large inlet a large proportion of droplets injected into the dryer become entrained in the upper recirculation zone that forms between the upper dryer walls and axial inlet jet. These droplets may remain in this hot zone for periods greater than 30 s, a significant time given that the residence time of the dryer is only 14.5 s (the dryer volume divided by the gas inlet flowrate). The behaviour of the droplets in the small throat simulation is quite different, with few droplets becoming entrained in the upper recirculation zone and most leaving the dryer within 10 s.

The different behaviour observed between the two simulations can be explained in terms of the gas and droplet momenta. In the small inlet simulation, the velocity of the gas at the position of the nozzle is high, with the result that droplets exiting the spray nozzle are accelerated quickly to the local gas velocity. Thus, these droplets remain near the most rapidly moving streamlines along the axis of the dryer and generally avoid entering the upper recirculation zone. In the large throat simulation, the gas velocity. As a result, droplets in this simulation end up in streamlines that are further from the axis of the dryer and are more likely to form part of the upper recirculation zone.

Even within the same simulation, the behaviour of each droplet is largely determined by its initial momentum. Since all droplets are injected into the chamber at the same speed in a given simulation, the initial droplet



Fig. 2. The trajectories of 100 sample droplets generated during the large throat $v_{\text{nozzle}} = 70 \text{ m/s}$ simulation, arranged in groups corresponding to different droplet diameters. The time scales have again been truncated. Taken from [29].

momentum is a function of the initial droplet size. Fig. 2 shows the trajectories of 100 sample droplets tracks produced during the above large throat simulation. The tracks are split into four groups based on initial droplet diameter. Droplets that have the smallest momentum relative to the gas, that is the smallest droplets, are accelerated most rapidly upon entering the dryer, and remain close to the centreline of the dryer throughout their life. As the droplet size increases however, droplets are accelerated to the local gas velocity at the nozzle at a decreasing rate, with the result that the larger the droplet, the more likely it is to become entrained in the upper recirculation zone and the longer it will spend in the chamber. This has implications in the drying of sensitive materials, such as milk, where too much time spent in the chamber (especially time spent near the hot air inlet) can lead to product degradation.

Wall deposition trends can also be explained in terms of the initial droplet and gaseous phase momenta. Fig. 3 shows where within the dryer droplets stick to the walls. To create this figure, the total height of the simulated dryer was segmented into 15 equally sized "bins", and the number of droplets that terminate in each bin when they stick to the dryer walls was accumulated. Results are shown from four simulations, three with the large inlet throat and a variety of initial droplet speeds, the fourth with the small inlet throat.

Fig. 3 shows that droplets stick to the walls in three main regions; the upper main chamber, the lower main chamber, and at the base of the bustle. It is not surprising that droplets impact the walls in these regions as these are the regions where flowfield streamlines are most tightly curved, that is, regions where droplets are most likely to traverse streamlines and impact with the walls. Case b of Fig. 3 (large throat simulation with the smallest initial droplet speed) has the lowest number of impacts within the lower main chamber and lower bustle regions, because the small momentum possessed by droplets after leaving the nozzle here results in trajectories that stay close to the axis of the dryer, that is, out of the high acceleration regions and away from the lower walls. As the initial droplet momentum is increased (Cases a and c of the figure), droplets follow streamlines that are further from the dryer axis, resulting in trajectories that run closer to the walls and a larger number of wall impacts in the lower region. The small throat simulation, Case d in Fig. 3, predicts that only a small number of droplets hit the dryer walls near the top of the main chamber. This is because, as explained



Fig. 3. Wall deposition as a function of elevation within the dryer. The z coordinate referred to in this figure lies along the centreline of the dryer and is directed upwards. Shown is the number of droplet tracks that terminate within each bin during each simulation, out of a total of 2000. Taken from [29].

previously, the increased momentum of the small diameter gas jet results in only a small proportion of droplets entering the upper recirculation zone.

3.2. Short form dryers

As explained earlier, the flow patterns and stability behaviour are very different in short form dryers, where the expansion ratio of the inlet geometry allows flow instabilities to develop. We have performed simulations for a wide range of dryers, ranging from simplified geometries used experimentally, through pilot scale dryers to full scale commercial dryers, as discussed below.

3.2.1. Laboratory-scale simulations

Experimental work in a scaled spray dryer chamber (900 mm in diameter and 2800 mm long) performed by Usi et al. [31] revealed the presence of an unsteady flow. Simulations performed using CFX4 by Guo et al. [32] were able to reproduce this behaviour. Fig. 4 shows a snapshot of an iso-surface of velocity showing the jet to be unsymmetrical and flattened, a result of the flapping motion occurring in the dryer.

This work is important in that it also revealed a significant difference in the behaviour of CFX4 and CFX5. CFX4 uses a segregated solver, based on the SIMPLEC algorithm, and in this geometry readily produces asymmetric behaviour leading to a periodic oscillating flow. CFX5 uses a coupled multi-grid solver and initially appeared to give a steady-state solution to this problem, in contrast with the experimental data. However, by running the solver for a significant elapsed time, jet instabilities appeared and the flow behaved just as in CFX4. A movie of the development of an iso-surface of velocity in the CFX5 simulation showed the very slow initiation of the instability. Our belief is that the coupled solver introduces much less "random noise" in the solution during the convergence process, as the simultaneous solution for the velocity components and pressure reduces significantly the error present at any stage in the iterative process. Therefore it takes significantly longer for an instability to grow to a critical amplitude, where the jet interaction with the walls then controls the flow behaviour. Instability initiation was seen to be favoured by using a large timestep initially, much larger than needed to resolve the instability. Once the instability appeared, the timestep was then reduced to properly resolve the transient flow. The coupled solver was then highly efficient at resolving the transient evolution of the instability.



Fig. 4. Iso-surface of velocity showing the geometry of the dryer and the flattened nature of the jet, resulting from the flapping motion.

3.2.2. Pilot-scale simulations

Southwell and Langrish [3] carried out extensive flow visualization studies on a pilot scale dryer (height 2 m, diameter 1 m) and, in particular, investigated the effect of the inlet swirl intensity on the flow behaviour. They observed large-scale, random sweeping motions outside the main air jet in the absence of swirl, which changed to much more directed motion when swirl was present. There was increased wall deposition in the swirling flow case. The geometry of the dryer used by Southwell and Langrish is shown in Fig. 5. We have simulated this dryer geometry and configuration using CFX5.6, and the results show the same flow characteristics [33]. Note in this case we found the transient instability developed readily if we started from a partially converged steady simulation and the grid was fine enough, typically composed of around 400,000 cells. A test case showed that a coarse grid gave a completely steady solution. These simulations were performed using the standard $k-\varepsilon$ model with wall functions. This choice was made based on our previous experience of sudden expansion flows (discussed earlier in Section 2.2) where even in the case of moderate swirl, the $k-\varepsilon$ model was found to predict the correct instability oscillation frequency.

Fig. 6 shows representative streamlines for inlet swirl angles of 0° , 15° and 25° cases. It is evident that in the 0° case there is a central jet with flow sweeping around the jet. These large scale vortices are observed to move with time. In the 15° case, the central jet has deflected towards the wall and there is a much more orderly motion in the outer region. This effect is increased further in the 25° case, and the more intense swirl within the dryer is evident. These simulations have shown the appearance of very complex jet behaviour, with a transition from a relatively stable jet through a single precessing central jet to a bifurcated jet that has very complex dynamical behaviour. Details of these simulations, including frequency spectra, velocity fields and comparisons with the observed flow behaviour are given elsewhere [33]. In addition, data are presented that show the complex flowfield that develops once vortex breakdown occurs and clearly illustrates why this regime is to be avoided in operating dryers.

It is worth noting that these gas only simulations were performed with CFX5, and using a 1 GHz two processor computer in parallel we were able to run simulations using one or two cpu days per case. This is a massive saving over earlier CFX4 simulations that required significantly longer run times.



Fig. 5. The geometry of the pilot scale dryer studied by Southwell and Langrish.



(c) 25° swirl angle case

Fig. 6. The effect of swirl angle on the flow behaviour as shown via streaklines starting from the inlet.

3.2.3. Plant-scale simulations

Several years ago we ran full transient simulation with transient particle tracking, hindered drying and wall deposition for an industrial scale dryer. These three-dimensional, transient simulations were extremely expensive computationally. For a real, commercial spray dryer with a 10 m diameter, 30 m height, 0.5 s of real time was simulated per day of CPU time on a 500 MHz DEC Alpha workstation with 1 Gb memory. This means that, as a routine on-line simulation tool, CFD is not a realistic prospect, and the computational speed needs to improve by five orders of magnitude for real-time simulations. CFD is, however, possible as an off-line optimization tool, but the requirement of around six weeks of CPU time for a single run (and several are required in any optimization) to produce a realistic simulated time period of interest is a significant limitation.

In gas flow only simulations, a precession frequency of around 1 Hz was observed. The simulations showed that the offset location of the dryer outlet pipe causes the centre of the precessing jet to be significantly off the

dryer axis. At certain times during the precession the jet was observed to come very close to the walls, so any droplets entrained in it would be very likely to hit the walls. In addition, a higher frequency precession was observed to be superposed on the 1 Hz motion but at that stage the simulations were not sufficiently well resolved to determine its detailed characteristics.

4. Conclusions and prospects

Simulation results presented here have shown that CFD models can play an important role in addressing both design issues and trouble-shooting in industrial spray dryers. The results show that simulation of fullscale dryers is now practical and can yield useful results. However, such computations are expensive, requiring significant run times for flow instabilities to develop and to settle to their quasi-steady limits, with run times of several days necessary for transient gas flow simulation.

A key issue in the study of short form dryers appears to be the resolution of the computational domain. We have shown that using coarse grids can suppress transient flow instabilities, even in three dimensions, whereas fine grid simulations and experimental data show clear precessing motion of the central air jet. Whilst it is tempting to use low resolution steady simulations, we have shown here that these do not reproduce the important flow phenomena and are misleading in the extreme. A dryer designed on steady simulations would predict minimal wall deposition, whereas we have seen that in certain flow regimes there would be very significant deposition.

We have already noticed that the move from CFX4, a block-structured, SIMPLE based CFD code to the unstructured, coupled solver of CFX5 has given significant benefits in terms of ease of setup and, more importantly, reduction of run times due to improved algorithms and efficient parallelization. Transient particle tracking is now available in ANSYS CFX (version 10.0) and the developed submodels of hindered drying and wall deposition are being migrated into this version of the code. On the basis of recent simulations, a significant reduction in run times is expected and, almost as important for industrial simulation, it offers much greater ease of use.

The simulations presented in this paper demonstrate that current CFD techniques are able to predict quite complex phenomena occurring in spray dryers, and highlight the potential of CFD in exploring the effect of gas and feed inlet parameters on flow stability, product quality and wall deposition rates. The key features of the modelling are the ability to run large-scale transient simulation that incorporate Lagrangian particle tracking and validated submodels of hindered drying and wall deposition.

Challenges for the future remain. Coalescence and agglomeration models need to be validated and included in the simulations. We have made much progress in this area and are continuing development work, but it is clear that a significant validation effort is needed before such models can be used with confidence. New turbulence modelling approaches, such as Detached Eddy Simulation (DES), are under investigation to determine their capabilities in this area. This progress relies on both continued model development and on-going experimental investigations to validate these models.

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