CFD SIMULATION OF HYDRODYNAMICS IN SPRAY DRYER

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CFD SIMULATION OF HYDRODYNAMICS IN SPRAY DRYER

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A thesis submitted in fulfillment of the requirements for the award of the degree of Bachelor of Chemical Engineering

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To my beloved family
&
my truly love

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ABSTRACT

Spray dryer is a well established method for converting liquid feed materials into dry powder forms. Spray dryer is widely used to produce foods such as whey, instant drinks, milk, tea and soups, as well as healthcare and pharmaceutical products, such as vitamins, enzymes, bacteria and also in production of fertilizers, detergent soap, and dyestuffs. Many experimental studies have been done to ensure the quality of the spray drying process. Alternatively, computational fluid dynamics (CFD) can be utilized to study the performance of the spray dryer. CFD modelling tools are increasingly used in the design, scale-up, optimization and trouble-shooting of the spray drying chamber because measurements such as Laser Droppler Anemometer (LDA) of air flow, temperature, particle size and humidity within the drying chamber are very difficult and expensive in a large scale spray dryer. Hydrodynamics of the spray dryer in single and multiphase flow are not well understood and hence for economic and safety reasons, reliable models are needed for scale-up and design of such a spray dryer. In this work, a CFD modelling of hydrodynamics in counter-current and co-current spray drying tower were performed. The turbulence modelling was realized using five different turbulent models, i.e. standard k-ε, RNG k-ε, Realizable k-ε, Reynolds stress models and the Detached Eddy Simulation. The predicted airflow patterns inside the spray drying chamber were found to be in good agreement to the experimental data adopted from literature for all turbulence models tested in this work. A great potential of the Detached Eddy Simulation for predicting the flow pattern in counter-current and co-current spray dryer were uncovered as its provides more accurate predictions compared to other models tested in this work. Results from this simulation may be useful for development of a more comprehensive and accurate model for spray dryer in the future.

ABSTRAK

Pengering semburan adalah keadah yang sangat baik untuk menukar bahan cecair menjadi serbuk kering. Pengering semburan banyak digunakan untuk menghasilkan makanan seperti serbuk dadih, minuman segera, susu, teh dan serbuk sup , begitu juga dengan produk kesihatan dan farmasi, seperti vitamin,enzim, bakteria dan juga di dalam penghasilan baja, sabun detergen, dan zat warna. Banyak kajian eksperimental telah dilakukan sebelum ini untuk memastikan qualiti proses pengering semburan. C*omputational fluid dynamics* (CFD) merupakan cara alternatif yang dapat dimanfaatkan untuk mempelajari prestasi alat pegering semburan ini. CFD semakin digunakan dalam reka bentuk, skala, optimasi and penyelesaian masalah pengering semburan kerana alat pengukur seperti *Laser Droppler Anemometer* (LDA) untuk mengukat aliran udara, suhu, saiz zarah, dan kelembapan dalam ruangan pengering adalah sangat sukar dan mahal untuk alat pengering sembur berskala besar. Hidrodinamik aliran fasa tunggal and multi tidak difahami dengan baik dan dengan untuk alasan ekonomi and keselamatan, model yang sewajarnya, amat diperlukan untuk skala dan reka bentuk pengering semburan. Dalam tugasan ini, pemodelan perolakan diwujudkan dengan menggunakan lima model perolakan berlainan dengan nama lain, *standard k-ε, RNG k-ε, Realizable k-ε, Reynolds stress models and the Detached Eddy* Simulasi. Pola aliran udara meramal dalam ruangan pengering semburan telah didapati bersamaan dengan data eksperimen yang diambil daripada kajian sebelumnya. Prestasi yang sangat baik oleh *Detached Eddy* Simulasi untuk meramal pola aliran di dalam pengering semburan aliran bertentangan dan aliran selari dapat ditemui menyediakan ramalan yang lebih tepat berbanding dengan model kajian yang lain dalam tugasan ini. Hasil daripada simulasi ini sangat berguna untuk pembanguanan dalam menghasilkan model yang lebih tepat dan menyeluruh untuk alat pengering semburan di masa hadapan.

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LIST OF ABBREVIATIONS/TERMINOLOGY/SYMBOLS

^{0}	-	Degree
2D	-	Two dimension
2^{nd}	-	second
3D	-	Three dimension
450k	-	Four hundred and fifty thousand
503k	-	Five hundred and three thousand
CFD	-	Computational Fluid dynamics
CPU	-	Central processing unit
DES	-	Detached Eddy Simulation
DPM	-	Discrete phase model
e.g.	-	for example
et al.	-	and others
hr	-	hour
i.e.	-	that is
K	-	Kelvin (Temperature)
k	-	Turbulent kinetic energy
kg	-	Kilogram
LDA	-	Laser Droppler Anemometer
LES	-	Large Eddy Simulation
m	-	meter
m^3	-	meter cubic
MF	-	Melamine-formaldehyde
Pa	-	Pascal (pressure)
PDA	-	Phase Doppler Anemometer
PIV	-	Particle Image Velocimetry
RANS	-	Reynolds-averaged Navier-Stokes

RKE	-	Realizable *k*-*ε*
RNG	-	Renormalized *k*-*ε*
RSM	-	Reynolds stress model
s	-	second (time)
SKE	-	Standard *k*-*ε*
UF	-	Urea-formaldehyde
VLES	-	Very Large Eddy Simulation
W	-	watt
ε	-	Turbulent energy dissipation rate

LIST OF APPENDICES

CHAPTER 1

1.0 INTRODUCTION

1.1 Motivation

Spray drying is a well established method for converting liquid feed materials into a dry powder form (Anandharamakrishnan *et al.*, 2007) by using hot gas steam. The water content in the feed materials is rapidly vaporized from the droplets, leaving particles of dry solid which are separated from the gas stream. The particles produced are light and porous. Spray dryer are widely used in food industries, such as production of whey and milk powder, in healthcare and pharmaceutical products such as enzyme and vitamins (Masters, 1991) and also production of fertilizers, detergent soap and dyestuff. All these productions are produce from different types of spray dryer.

Gas flow pattern is one of primary factor that influence the quality of the product by spray dryer. The internal gas flow pattern directly influences the residence time each droplet or particle spends within the dryer, and the temperature of the gas which surrounds the particle during this period. These parameters affect the moisture content, size distribution, and porosity of the final product (Harvie *et al.*, 2001).

In recently year, to ensure the quality of the spray dryer production, there were a lot of experimental had been done. The quality of the product from spray dryer processes can be determine by using advanced method such as Laser Doppler Anemometer (LDA) and Phase Doppler Anemometer (PDA). However this measurement equipment still has their limitations. The LDA and PDA techniques were difficult and very expensive in large scale spray dryer. Alternatively, CFD can provide detail description on the multiphase flow in spray dryer which is certainly much cheaper to run compare to experiment. CFD modelling tools are increasingly used in the design, scale-up, optimization, and trouble-shooting of spray dryer (Anandharamakrishnan *et al.*, 2007).

1.2 Objective and scope

The aim of this study is to develop a modelling method for predicting single phase and multiphase hydrodynamics in spray dryer chamber to make possible the modelling spray drying via CFD. The first part of this work dealing with the modelling of single phase spray dryer were carried out to evaluate the performance of various turbulence models namely standard k-ε (SKE), RNG k-ε (RNG), Realizable k-ε (RKE), RSM and Detached Eddy Simulation (DES) and this study cover the axial and tangential velocity flow in a spray dryer at several positions. The second part involves the development method for multiphase flows which i.e. spray drying of maltodextrin. The Discrete phase model (DPM) was selected with energy balances equation to give the prediction of simultaneous heat and mass transfer during the drying process. Two different case study was performed as follow using FLUENT 6.3 CFD package.

Case A: Counter-current spray dryer simulation using the geometry and boundary conditions studied by Bayly *et al.* (2004).

Case B: Co-current spray dryer simulations using geometry and boundary conditions studied by Kieviet (1997).

1.3 Main contribution of this work

The Detached Eddy Simulation (DES) employed to solve a turbulence flow in a single and multiphase flows spray dryer in this work is relatively new and has not been previously applied to solve for a spray dryer. It is important to develop a method that can be employed by designers or practical engineers as an exploratory design and scale-up tools. To predict the performance of spray dryer accurately, must be able to model the flow pattern in spray dryer (Harvie *et al.*, 2001). In the past, modelling of gas flow pattern was limited comparison of turbulence models prediction on hydrodynamics of complex spray dryer design such as counter-current spray dryer tower. The previous CFD studies either under or over predicts the experimental data due to shortcomings of the turbulence model used.

Therefore, the Detached Eddy Simulation (DES) was employed to solve the turbulence model in single and multiphase in spray dryer in this work. Further detail about the DES is given in section 3.5.1. DES model is belonged to hybrid turbulence models, which blend Large Eddy Simulation (LES) away from the boundary layer and RANS near the wall. This marks a significant improvement in spray dryer modelling, which enable a direct comparison with LDA experimental data.

1.4 Thesis outline

The structure of the reminder of the thesis is outlined as follow:

Chapter 2 provides applications and general features of the spray dryer. A general description on the flow characteristics in spray drying chamber and correlations to account for the flow phenomena are presented. This chapter also provides a brief discussion about the previous work related to advanced experimental techniques available for spray dryer, mentioning their applications and limitations for gas flow pattern analysis.

Chapter 3 will present the solution procedures about the spray dryer modelling dimension and set-up and also give a detail of the computational approach applied for spray dryer modelling of single and multiphase flows including the turbulence modelling, computational grid, and particle heat and mass transfer model for multiphase flow and solution procedures. The mathematical model used to account for turbulence flow of single and multiphase system is also described.

In chapter 4 provides the result and discussions of the simulations prediction of spray dryer. The performance of four different RANS model and a DES model turbulence model were compared with experimental data.

In chapter 5, as the last chapter has been concluding all together the summary and have a recommendation for the future study of spray dryer modelling.

CHAPTER 2

2.0 LITERATURE REVIEW

2.1 Overview

This chapter gives a brief description of the system and applications of spray drying in industry. In addition, the experimental techniques used to determine the hydrodynamics in spray dryer are also described. A brief summary about the experimental data available from literature and adopted for comparison with CFD simulation is also presented. This chapter also provides a summary of the previous experimental work on spray drying.

2.2 Introduction

Drying is a process to removal of other organic liquids, such as benzene or organic solvents from process materials. Most of the drying processes are concerned with removal of water content from solid particles. This technique is the oldest method of preserving food such as for grapes, corn, and meat. Until now, drying processes is an indispensable in many food industries.

According to Okos *et al.* (1992), the goals of drying process research especially in food industries are three-fold; (1) Economic considerations: to reduce cost and improve capacity per unit amount of drying equipment, to develop simple drying equipment that is reliable and requires minimal labour, to minimize off-specification product and develop a stable process that is capable of continuous operation, (2) Environmental concerns: to minimize energy consumption during the drying operation and reduce environmental impact by reducing product loss in waste streams, and (3) product quality aspects: to have precise control of the product moisture content at the end of the drying process to minimize chemical degradation reactions, to reduce change in product structure and texture, to obtain the desired product color, to control the product density and to develop a flexible drying process that can yield products of different physical structures for various end user. Types of equipment of drying process which are commonly use are tray dryer, vacumm-shelf indirect dryer, continuous tunnel dryer, rotary dryers, drum dryer drying of crops and grains and the very well establish spray drying.

2.3 Application of spray drying

In a spray drying a liquid or slurry solution is sprayed into a hot gas steam and converting the liquid feed to the form of a mist of fine droplets. The water is rapidly vaporized from the droplets, leaving particles of dry solid which are separated from the gas steam. The particles produced are light and porous. Spray drying is widely used in produce food, as well as healthcare and pharmaceutical products (Masters, 1991) also in production of chemical and polymer.

2.3.1 Food industry

Production of food such as instant coffee, milk powder, soup mixer, Maltodextrin, herbs extracts and vegetable protein via spray drying is very ideal due to heat sensitive products, where selection of system and operation is the key of high nutritive and quality powder of precise specification. Short form co-current spray dryer with a bottom outlet is more suitable for drying heat sensitive products (Anandharamakrishnan *et al.*, 2007).

2.3.2 Healthcare and pharmaceutical industry

The production of healthcare and pharmaceutical such as vitamins, enzymes, antibiotics, and vaccines was produced by spray dryer. Spray dryer designed specially for integration into batch or continuous operations under sanitary or aseptic conditions. This system is available for taste masking and encapsulation. Dryers with integrated fluid beds are ideal for producing non-dusty powders for perfect tablet form.

2.3.3 Chemical industry

Spray dryers for chemical industries produce a variety of powdered, granulated and agglomerated products in systems that minimize formations of gaseous, particulate and liquid effluent. The production from Chemical industry such as catalyst, detergent, dyestuffs, and inorganic chemicals for drying more robust materials the counter-current process offers higher thermal efficiency and can lead to different, in some desirable, products characteristics (Bayly *et al.*, 2004).

2.3.4 Polymer industry

The polymer production such as e-PVC and UF/MF resins, polymer dispersions and solutions in water or organic solvents are spray dried under closed controlled operating condition, producing powders to precise particle size, heat treatment, and redispersibility specifications. Low softening point products are produced continuously in plants with air-brooms, air sweeps or integrated fluid bed.

It is clear shown above, from the example and explained above the spray drying are widely used in the process industries. All the production involves different types of spray drying depend on production characteristic.

2.4 Experimental methods for spray drying

The focus of this study is on development of computational tools to design spray drying. Nevertheless, it is important to review the experimental techniques that are available and which provide validation data for single and multiphase flow

CFD prediction. There are several advanced techniques of measurement the flow phenomena in spray drying chamber. Among them are microseparator, Particle Image Velocimetry (PIV), Laser Doppler Anemometry (LDA) and Phase Doppler Anemometry (PDA).

2.4.1 Microseparator

The microseparator is a device for temperature and humidity measurement, developed by Kieviet and Kerkhof (1996).

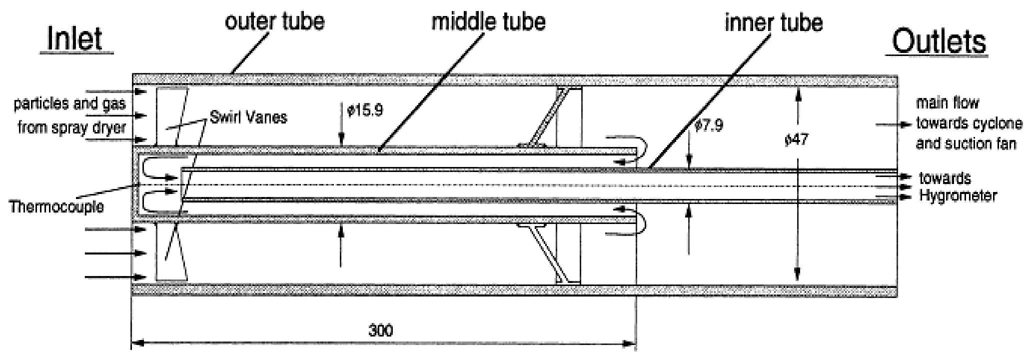


Figure 2-1: Concept of microseparator device

This device separates small particles from the gas flow by means of the difference in inertia between the fluids and the particles. Two mechanisms of separation are employed successively, namely a swirling motion and a sharp change in direction of the flow. A small fraction of the clean air flow is then directed to a thermocouple and subsequently to a dew-point hygrometer (Kock *et al.*, 2000).

2.4.2 Particle Image Velocimetry

Particle Image Velocimetry (PIV) is a non-intrusive laser optical measurement technique for research and diagnostics in hydrodynamics flow. PIV is very common and useful tool to investigate the flow phenomena in spray dryer models, there is a need to measure droplet velocities, cone angles, penetration length etc. Another used for investigated the flow phenomena in blood vessels, heart valves or artificial organs. A 2D high-resolution PIV system has been developed, setup and successfully tested. The system contains a high speed video camera for the image capture and a continuous laser light source with adapted light sheet optics for the illumination of the flow. After recording the images are stored to the hard disk drive of a PC and can be analyzed using correlation technique. In this area, the development of more powerful PIV looks very promising (Kieviet, 1997). To enhance the understanding of the flow phenomena of wet granular flows and provide a knowledge-based approach to improve spray driers in terms of stability.

2.4.3 Laser Doppler anemometry/Phase Doppler anemometry

LDA/PDA is another non-intrusive single point optical technique applicable for the simultaneous measurement of particle size distributions and gas velocities. Both LDA and PDA have similar working principle except for a simultaneous measurement of particle velocity and size distribution capability in PDA. PDA was said to an extension of the LDA principle (Dantec dynamics, 2009). In LDA/PDA technique two laser beams are focused into a small measurement volume where they produce interference fringes. The laser light is scattered when a particle passes through the measurement volume. The seed particle act as moving light sources causing Doppler shifts of the scattered light. The Doppler shift of the lights is proportional to the bubble velocity while the phase differences between the lights scattered in different directions are linearly related to the particle size. This technique which is enables the velocity of the seeded particles 0.5-5 microns in air.

2.5 Experimental studied on Spray drying

Many experimental and numerical studied have been performed for spray drying to ensure the quality of product of the spray drying processes (Kieviet *et al.*, 1997; Southwell and Langrish, 2000; Harvie *et al.*, 2002; Zbicinski *et al.*, 2002; Bayly *et al.*, 2004; Langrish *et al.*, 2004; Huang *et al.*, 2005; Anandharamakrishnan *et al.*, 2007). Some of the most significant work is summarized in Table 2-1. Prediction from earlier work is less accurate due to shortcoming of turbulence model and most of studies focus on 2D axi-symmetric. For example, previous research by Kieviet (1997) which have cover the experimental and CFD modelling of short co-current spray dryer. Kieviet (1997) was compared the experimental data with CFD codes FLOW3D used Standard k-ε turbulence model in 2D axi-symmetric. His results cannot give a realistic primary particle residence times as swirl and recirculation were not fully considered (Anandharamakrishnan *et al.*, 2007). Research by Bayly *et al.* (2004) in studied the airflow patterns in a counter-current spray drying tower by compared the simulation of RSM model study with LDA experimental data. The result either under or over predicts the experimental data which may be attributed by the use of RANS model to account for a strongly anisotropic flow in counter-current spray dryer tower. Such a flow may be better modeled using a hybrid RANS-LES model i.e. DES which well be evaluated in this work.

Table 2-1: Experimental and numerical study on spray drying

AUTHOR	EXPERIMENT			MODELLING			REMARK
	Humidity	Temperature	Velocity	Humidity (H)	Temperature	Velocity	
Zbicinski *et al.* (2002)	Microseparator		Laser Doppler Anemometry	No	No	No	Advanced experimental technique needed to determine current parameters of spray drying process in full scale tested.
Harvie *et al.* (2001)	No	No	No	No	No	Very Large Eddy Simulation (VLES)	In order to gain a more detailed understanding of the flow patterns and their stability in counter-current spray dryer.
Harvie *et al.* (2002)	No	No	No	No	No	CFX4.3, standard *k-ε*	Found that the behavior of the dryer is largely determined by the relationship between the initial of the injected particles and gas flow within the dryer
Huang *et al.* (2006)	No	No	No	CFX, Hybrid Eulerian and Lagrangian approach, RNG *k-ε* turbulence model, 3D			A 3D CFD model is more suitable for such spray drying system than 2D axi-symmetric model.

Table 2-1: Experimental and numerical study on spray drying (Continued)

AUTHOR	EXPERIMENT			MODELLING			REMARK
	Humidity	Temperature	Velocity	Humidity	Temperature	Velocity	
Mezhericher *et al.* (2008)	No	No	No	CFD package FLUENT 6.3.26 Eulerian approach Lagrangian approach Standard *k*-*ε* model 2D			The droplet collisions have a marked influence on temperature and humidity pattern.
Mezhericher *et al.* (2009)	No	No	No	Steady-state and unsteady state 2D axisymmetric and 3D Eulerian -Lagrangian approach Standard *k*-*ε* model			2D model is suitable for fast and low-resource consumption numerical calculations and it prediction for velocity, temperature and humidity eith reasonable accuracy. However 2D failed to predict flow pattern and cannot provide picture of particle trajectories but can by utilized 3D model.

Table 2-1: Experimental and numerical study on spray drying (Continued)

AUTHOR	EXPERIMENT			MODELLING			REMARK
	Humidity	Temperature	Velocity	Humidity	Temperature	Velocity	
Kieviet (1997)	Microseparator		Hot wire probe	CFD codes FLOW3D Standard *k*-*ε* model 2D axi-symmetric			Hot-wire probe cannot function with a spray present. Airflow, temperature, and humidity pattern can be calculated by tracking the evaporating particle through the microseparator measurement. CFD is to gain better understanding in the processes taking place.
Bayly *et al.* (2004)	No	No	Laser Doppler Anemometry	No	No	Reynolds Stress model	RSM turbulence model shows good prediction with comparison of experimental data
Anandharamakhrishnan *et al.* (2007)	No	No	No	CFD code FLUENT 6.3 Discrete phase model (DPM) Standard *k*-*ε* model			3D model is more suitable for analyzing a spray drying system than a 2D axi-symmetric model.

Table 2-1: Experimental and numerical study on spray drying (Continued)

AUTHOR	EXPERIMENT			MODELLING			REMARK
	Humidity	Temperature	Velocity	Humidity	Temperature	Velocity	
Huang *et al.* (2004)	No	No	No	No	Standard *k-ε*, Realizable *k-ε*, RNG *k-ε* and RSM turbulence models		Prediction of RNG *k-ε* model performs better in the specific case. (Spray dryer fitted with a Rotary Disk Atomizer
Le Barbier *et al.* (2001)	No	No	No	No	No	CFD model CFX5 Navier Stokes	Spray dryer was strongly time-dependent, the *k-ε* turbulence model on suitably resolved numerical grid, is suitable for estimating the frequencies of precession in spray dryers.
Huang *et al.* (2006)	No	No	No		CFX codes RNG model 3D Hybrid Eulerian and Lagrangian approach		Shows that the 3D modle is more suitable for such a spray drying system than 2D axi-symmetric model.

2.6 Summary

The system and application of spray dryer have been outlined in this chapter. From the description above, shows the different types of spray dryer i.e. counter-current and co-current spray dryer are very well establish equipment involve widely in industries such as production of milk powder in food industry and production of detergent powder from chemical industry. Many experimental studied have been done to unsure the quality of the spray drying processes for example research by Kieviet (1997) and Zbicinski *et al.* (2002). The advanced techniques measurements have been used for this purpose; however those advanced measurements have limitation because, measurements of air flow, temperature, particle size and humidity within the drying chamber are very difficult and expensive in large scale spray dryers (Anandharamakrishnan *et al.* (2007). Alternatively, computational fluid dynamics (CFD) can be utilized to study the performance of the spray dryer. Many studied have been undertaken in the past to compare the CFD result and experimental measurement for single phase and multiphase flow in spray dryer. In most cases, only focuses on using Reynolds Averaged Navier-stokes turbulence model to study the flow pattern inside the drying chamber (Harvie *et al.*, 2001; Huang *et al.*, 2006; Bayly *et al.*, 2004; Anandharamakrishnan *et al.*, 2008). Several researchers (e.g. Zbicinski *et al.*, 2002; Bayly *et al.*, 2004; Kieviet, 1997) had carried out detail measurement on the single and multiphase flow in spray dryer chamber. In this work, the CFD simulation of RANS and DES turbulence model for single phase flow is compared to LDA experimental measurement from Bayly *et al.* (2004) for counter-current spray dryer. Whereas results from multiphase flow CFD simulation is compared to Kieviet (1997) experimental data for co-current spray dryer. The DES turbulence models have never been previously used for modelling of spray drying and its performance for predicting the single and multiphase flow in spray dryer is evaluated in this work.

CHAPTER 3

3.0 COMPUTATIONAL APPROACH

3.1 Overview

This chapter mainly presents the solution procedures about the spray dryer modelling dimension and set-up and also the computational approach applied for spray dryer modelling of single and multiphase flows including the turbulence modelling, computational grid, and particle heat and mass transfer model for multiphase flow. The mathematical model used to account for turbulence flow of single and multiphase system is also described. In the CFD approaches the Detached Eddy Simulation (DES) employed in this work is based on the Spalart-Allmaras turbulence model and four Reynolds-averaged Navier-Stokes (RANS) models, namely standard k-ε (SKE), realizable k-ε (RKE), renormalized k-ε (RNG) and Reynolds stress model (RSM) were evaluated on this study and all the turbulence model were solved on a grid containing about (503k) for counter-current spray dryer and about (450k) control volumes for co-current spray dryer.

3.2 Introduction

Spray dryers are widely used in the food industry such as production of whey, milk powder, soup mixer and coffee and also in chemical, polymer, and pharmaceutical industrial production. The spray dryers usually take part at the end of the product processes which to convert the liquid product to particle or droplet form. The flow phenomena inside the drying chamber are of great importance in the design, scale-up and optimization of spray dryer which will effect to the quality of the spray dryer product. Although several advanced method such as LDA and PDA are capable of evaluating the flow phenomena in spray dryer, these method still have their own limitations because, measurements of air flow, temperature, particle size and humidity within the drying chamber are very difficult and expensive in large scale spray dryers (Anandharamakrishnan *et al.* (2007). Alternatively, the CFD provides a powerful tool for investigating flows at lower expense than would be required by a high quality experimental facility. However, attention should be paid to evaluate the level of accuracy offered by CFD on the prediction of turbulent flows in spray dryers.

Simulation of the single phase and multiphase phase spray dryers especially for counter-current spray dryer tower is necessary because there are still a lot of discussions and arguments related to the prediction of turbulent flows in spray dryer. As mention before, to predict the performance of spray dryer accurately, must be able to model the flow pattern inside the dryer chamber (Harvie, 2001).

It is possible to solve the turbulence flow in spray dryer without any modelling. This problem can be solving by using measurement detector such as LDA and PDA. However, these methods are very difficult and expensive in large scale spray dryer (Anandharamakrishnan *et al.*, 2007). Modelling of turbulence in spray dryers is challenging because the flow inside the dryer chamber are highly three-dimensional and recirculation of unsteady RANS flow are fully considered.

Many researchers (Kieviet, 1997; Harvie *et al.*, 2002; Huang *et al.*, 2006; Bayly *et al.*, 2004; Anandharamakrishnan *et al.*, 2007; Mezhericher *et al.*, 2008) have studied Reynolds averaged Navier-Stokes (RANS) based turbulence models (mainly standard k-ε models) applied to a spray dryer. As a general conclusion, the authors claim that the CFD predicts satisfactorily the axial and radial mean flow patterns, but either under or over prediction of the tangential velocity component and turbulence quantities, such as the turbulent kinetic energy (k) and turbulent energy dissipation rate (ε). Fletcher *et al.*, (2006) noted that, turbulence modelling in three – dimensional in nature is very important for design purposes. Research by Bayly *et al.*

(2004) employed RSM turbulence model in their work and it seems to give a good prediction of the swirling flow inside the spray dryer. However, there still discrepancy especially on the prediction of gas axial velocity as shown in Figure 3.1, whereas shows under prediction in comparison to the measurement from the experimental result.

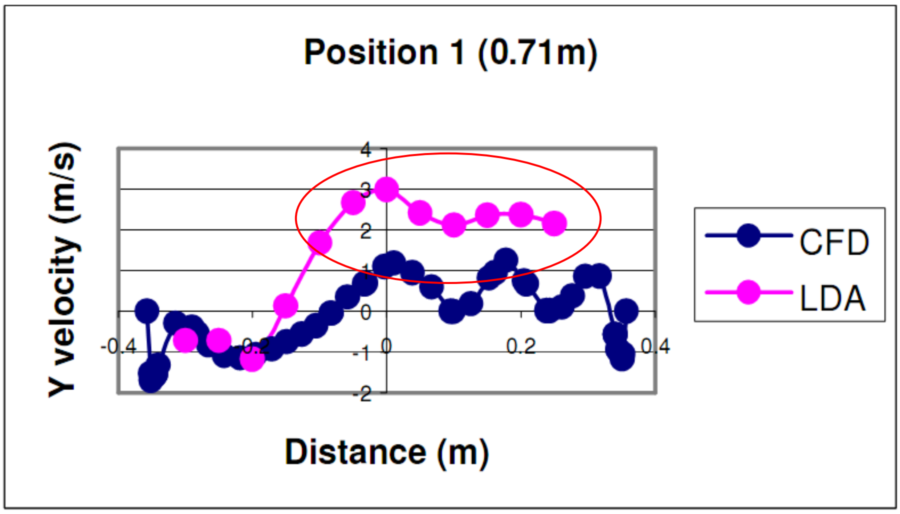


Figure 3-1: Axial velocity result from Bayly *et al.* (2004)

The main issues about the modeling of spray dryer by using the RANS turbulence models give poor prediction of the turbulence related quantities i.e. *k*, *ε* and mean velocity. Besides, these models need more CPU time and large memory required to resolve the effects of sub-grid scale eddies. Such problem led to the idea of formulating a turbulence model that is cheaper to run and has a better prediction of turbulent flow called DES or hybrid (RANS-LES) turbulence model. The main idea of this model is to combine RANS modeling with LES for applications in which classical LES is not affordable i.e. at boundary layer. For boundary layer at high Reynolds number, LES may not yield sufficient resolution of the near wall flow structure because large eddies close to the wall are physically small scale (Squires *et al.*, 2005) and also non-isotropic. Thus LES model need very fine grid within the boundary layer, which means the computational cost of the whole domain does not differ appreciably from DNS (Spalart *et al.*, 1997). Therefore, DES was invented by Spalart *et al.* (1997) in attempt to reduce the computational cost, as well as to provide a good prediction of turbulence flows near the boundary layer. DES reduces to a RANS model in the boundary layer, thus permitting a coarser grid than a conventional LES grid, resulting in fewer grid cells overall and faster computational. To the author knowledge, DES has never been used previously for prediction of spray dryer flows.

The overall research methodology consists of two main steps. First step is about drawing the spray dryer geometric and set the set-up and for the second step is about analysis the flow in spray dryer tower as in Figure 3.2 below.

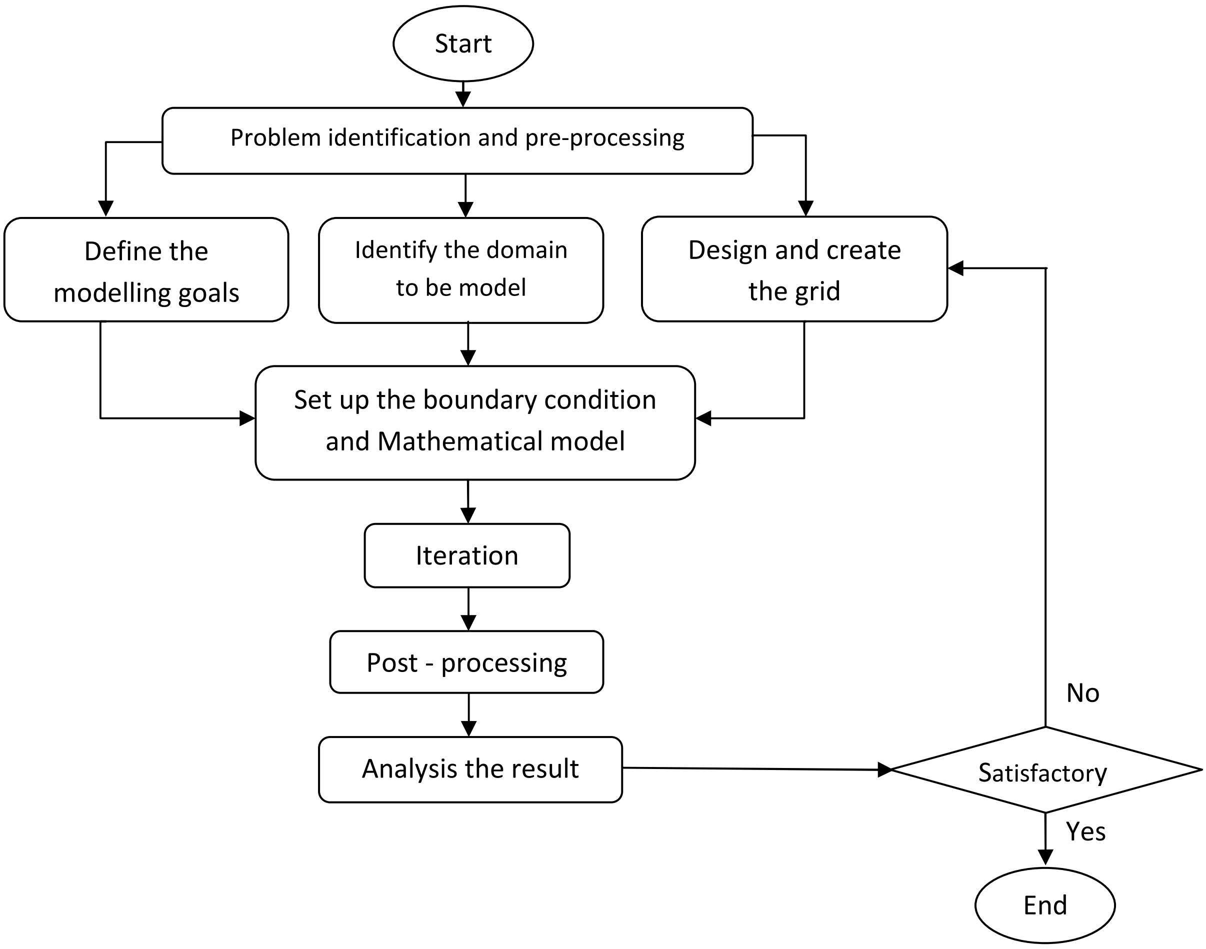
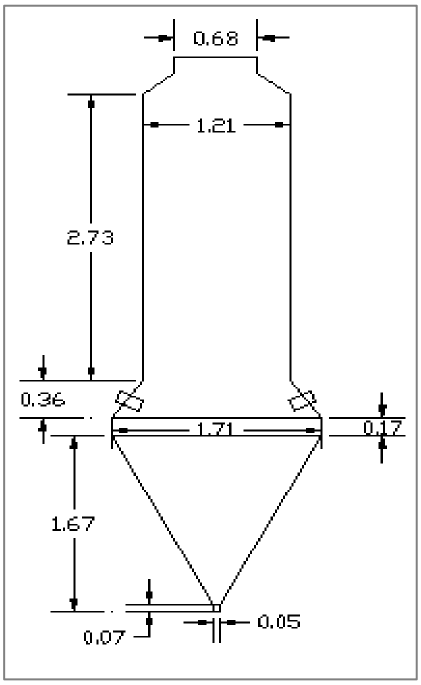


Figure 3-2: Steps on CFD analysis

3.3 Case A: Counter-current spray dryer

The commercial CFD code, FLUENT 6.3, was used to simulate the three-dimensional configuration of a counter current spray dryer tower fitted with eight main inlets set around the tower hip. This spray dryer model consists of two inlets, the main inlet and the based inlet. The main inlet cylinder shape was set at 25^0 below the horizontal and 25^0 to the radius in the horizontal plane which imparting a significant swirl to the flow in the tower. GAMBIT software, version 6.2.4 was used to draw the spray dryer tower diagram illustrated in Figure 3.3, which has same dimension to the one studied by Bayly *et al.* (2004).



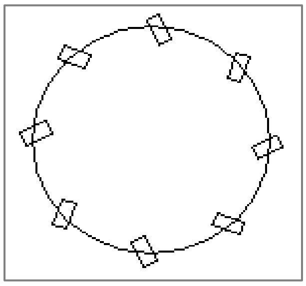


Figure 3-3: Counter-current spray dryer geometry (right) and the main inlet position (left)

The main inlet was set as the porous zone; with the fluid porosity is about 0.295. The outlet on the top of the spray dryer tower is set as outflow at specify boundary. In order to study the grid dependent in this work, the simulation was performance using counter current spray dryer composed mainly consisting about (503k) hexahedral and tetrahedral cells. The boundary layer and size function tools were used to make sure the grid created sufficiently resolve the flow around boundary layer and hence minimizing the simulation error.

The total air flow through the eight main inlets to the tower is 3814 m^3/hr and for the based inlet air flow is 239m^3/hr. This work attempt to evaluate the performance of various Reynolds-averaged Navier-Stokes (RANS) based turbulence models namely which is standard *k-ε* (SKE), RNG *k-ε* (RNG), Realizable *k-ε* (RKE), Reynolds stress models (RSM) and the Detached Eddy Simulation (DES) model. The SIMPLE (semi-implicit pressure linked equation) method was used for the pressure-velocity coupling and 2^{nd} order differencing for momentum terms for the RANS modelling, whereas the bounded central differencing was used for DES simulation. This simulation was performed using the unsteady solver.

3.4 Case B: Co-current spray dryer

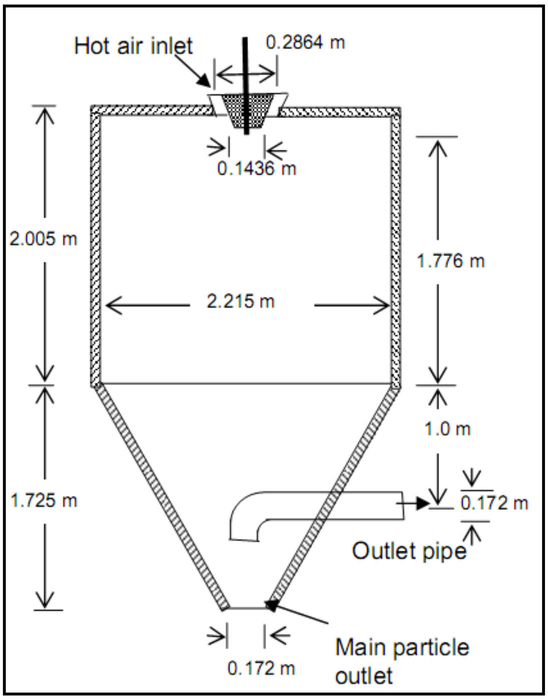


Figure 3-4: Co-current spray dryer geometry

The other case has simulated dimension to the one studied experimentally by Kieviet (1997) and numerically by Anandharamakrishnan *et al.* (2007) and Huang *et al.* (2006).

Table 3-1: Boudary conditions used for co-current spray dryer simulation

Inlet Air		
Air inlet temperature	468	(K)
Air mass flow rate	0.336	(kg/s)
Air total velocity	9.15	(m/s)
Outlet condition		
Outflow and reference at outlet	-100	(Pa)
Turbulence inlet condition		
Turbulence k-value	0.027	(m^2/s^2)
Turbulence ε-value	0.37	(m^2/s^2)
Liquid spray from nozzle		
Liquid feed rate (spray rate)	0.0139	(kg/s)
Feed temperature	300	(K)
Spray angle	76^0	
Chamber wall conditions		
Chamber wall thickness	0.002	(m)
Wall material	Steel	
Overall wall-heat transfer co-efficient	3.5	(W/m^2K)
Air temperature outside wall	300	(K)
Interaction between wall and droplet	escape	

The SIMPLE (semi-implicit pressure linked equation) method was used for the pressure-velocity coupling and 2nd order differencing for momentum terms for the standard *k-ε* modelling, whereas the bounded central differencing was used for

DES simulation. The discrete phase model (DPM) was applied for prediction of multi phase flow. This simulation was performed using the unsteady solver. The data presented in this work were taken as a statistical average from up to 1000 time step after the pseudo convergence was achieved.

3.5 CFD approach for spray drying

3.5.1 Turbulence modelling

The selection of turbulence model for spray dryer simulations is very important, especially when dealing with higher Reynolds numbers and presented of swirling flows. Comparatively new turbulence models such as DES need to be validated further before they can be applied routinely to spray dryer modeling. It is also interesting to explore in detail the strength and weakness of the currently available RANS models, whem dealing with swirling flows in spray dryer. Therefore the predictive capabilities of four RANS models, namely standard *k*-*ε* (SKE), *k*-*ε* (RNG), Realizable *k*-*ε* (RKE), Reynolds stress models (RSM) as well as DES, on turbulent flows in a single phase and multiphase have been extensively compared in this study. These models are described in more detail below.

The standard *k*-*ε* model is a semi-empirical model based on transport equations for the turbulent kinetic energy and its dissipation rate. Transport equations for *k* and *ε* for all *k*-*ε* variant models can be generalised as follow:

$$\underbrace{\frac{\partial(\rho k)}{\partial t}}_{\text{time derivative}} + \underbrace{\frac{\partial}{\partial x_i}(\rho u_i k)}_{\text{convection}} = \underbrace{\frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right)}_{\text{diffusion}} + \underbrace{\rho P_k}_{\text{production}} - \underbrace{\rho \varepsilon}_{\text{destruction}} \tag{3-1}$$

And

$$\underbrace{\frac{\partial(\rho \varepsilon)}{\partial t}}_{\text{time derivative}} + \underbrace{\frac{\partial}{\partial x_i}(\rho u_i \varepsilon)}_{\text{convection}} = \underbrace{\frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right)}_{\text{diffusion}} + \underbrace{S_\varepsilon}_{\text{source term}} \tag{3-2}$$

The turbulent (eddy) viscosity, μ_t, is obtained from:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{3-3}$$

The relation for the production term, P_k, for the *k*-*ε* variant models (i.e. *k*-*ε*, RKE and RNG) is given as:

$$P_k = \mu_t \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} \tag{3-4}$$

For the standard *k*-*ε* model the source term, S_ε, is given by:

$$S_\varepsilon = \rho \left(C_{1\varepsilon} \frac{\varepsilon}{k} P_k - C_{2\varepsilon} \frac{\varepsilon^2}{k} \right) \tag{3-5}$$

The model constants are (Launder and Spalding, 1974): $C_{\varepsilon 1} = 1.44$ $C_{\varepsilon 2} = 1.92$ $C_\mu = 0.09$ $\sigma_k = 1$ $\sigma_\varepsilon = 1.3$ derived from correlation of experimental data.

As the strengths and weaknesses of the standard *k*-*ε* model have become known, improvements have been made to the model to improve its predictive capability, leading to an introduction of variants such as the RKE model, which was first introduced by Shih *et al.* (1995). The RKE model is said to be a substantial improvement over the standard *k*-*ε* model, as it consider flow features such as strong streamline curvature, vortices and rotation. RKE differs from the standard *k*-*ε* model in two important ways: first it has a new formulation of the turbulent viscosity and second it employs a new transport equation for the dissipation rate. RKE still has a similar equation for μ_t as *k*-*ε*, but C_μ is no longer a constant and instead is a function of velocity gradients given as:

$$C_\mu = \frac{1}{A_o + A_s \frac{U^* k}{\varepsilon}} \tag{3-6}$$

with A_o = 4.04, $A_s = \sqrt{6}\cos\phi\,;\phi = \frac{\cos^{-1}\left(\sqrt{6}w\right)}{3}, w = \frac{S_{ij}S_{jk}S_{ki}}{\tilde{S}^3}$, $U^* = \sqrt{S_{ij}S_{ij} + \tilde{\Omega}_{ij}\tilde{\Omega}_{ij}}$ and $\tilde{S} = \sqrt{S_{ij}S_{ij}}$ to ensure positivity of normal stresses ($\overline{u_i^2} \geq 0$) and Schwarz's inequality for shear stress ($(\overline{u_i u_j})^2 \leq \overline{u_i^2}\ \overline{u_j^2}$). The Schwarz inequality for shear stresses in *k*-*ε* model can be violated when the mean strain rate is large, but it can be eliminated by having a variable C_μ (Fluent 6.2, 2005).

The source term, S_ε for RKE is now given as:

$$S_\varepsilon = \rho\left(C_1 S\varepsilon - C_2 \frac{\varepsilon^2}{k + \sqrt{\upsilon\varepsilon}}\right) \tag{3-7}$$

The model constants are (Shih *et al.*,1995): $C_1 = \max\left[0.43; \frac{\eta}{\eta + 5}\right]$, $C_2 = 1.9$, $\sigma_k = 1$ and $\sigma_\varepsilon = 1.2$ with $\eta = Sk/\varepsilon$, and $S = \sqrt{2S_{ij}S_{ij}}$ is a modulus of mean rate of strain tensor.

The RNG model was obtained from renormalization group theory by Yakhot and Orzag (1986). RNG differs from standard *k*-*ε* because it has an additional term, *α*, in the *ε* transport equation, besides providing an analytical formula for the turbulent Prandtl numbers derived using RNG theory. Thus the source term S_ε for RNG is given by:

$$S_\varepsilon = \rho\left(C_{1,RNG} \frac{\varepsilon}{k} P_k - \sigma^{-1}\frac{\varepsilon^2}{k} - C_{2,RNG}\frac{\varepsilon^2}{k}\right) \tag{3-8}$$

where σ^{-1} is the inverse effective Prandtl number given by

$$\sigma^{-1} = \frac{C_\mu \eta^3 (1 - \eta/\eta_0)}{1 + \beta\eta^3} \tag{3-9}$$

Instead of a constant value for the turbulent Prandtl number in *k*-*ε*, it is provided analytically in RNG by the following equation:

$$\left|\frac{\sigma^{-1} - 1.3929}{\sigma_0^{-1} - 1.3929}\right|^{0.6321} \left|\frac{\sigma^{-1} - 2.3929}{\sigma_0^{-1} - 2.3929}\right|^{0.3679} = \frac{\mu_{mol}}{\mu_{eff}} \tag{3-10}$$

where σ_0^{-1} = 1.0. In the high Reynolds number limit (μ_{mol} /μ_{eff} << 1), the inverse turbulent Prandtl number is $\sigma_{k\cdot}^{-1}$= σ_ε^{-1} ≈ 1.393.

The RNG model uses a term called the effective viscosity for a flow at low Reynolds numbers, but it is not relevant in the current work, which is in the fully turbulent region (Re > 20000). The effective viscosity is modelled as eq. (3) for the RNG model at high Reynolds number (Fluent 6.2, 2005). Similar to the RKE model, $\eta = Sk/\varepsilon$, and $S = \sqrt{2S_{ij}S_{ij}}$ is a modulus of mean rate of strain tensor, $\eta_0 = 4.38$, $\beta = 0.012$. The model constants are $C_{\varepsilon 1} = 1.42$, $C_{\varepsilon 2} = 1.68$, $\sigma_k = 1.393$, $\sigma_\varepsilon = 1.393$ derived from RNG theory by Yakhot and Orzag (1986).

RSM abandons the assumption of the isotropic eddy-viscosity hypothesis, to close the Reynolds-averaged Navier-Stokes equations, by solving transport equations for the individual Reynolds stresses, together with a transport equation for the dissipation rate. RSM has a greater potential to give accurate predictions for complex flows, as it takes into accounts the effects of streamline curvature, swirl, rotation, and rapid changes in strain rate in a more rigorous manner than two-equation models such as *k*-*ε*. The foundation of RSM is the exact set of transport equations:

$$\underbrace{\frac{\partial}{\partial t}\left(\rho\overline{u_i'u_j'}\right)}_{\text{Time derivative}}+\underbrace{\frac{\partial}{\partial x_k}\left(\rho u_k\overline{u_i'u_j'}\right)}_{C_{ij}=\text{Convection}}=\underbrace{-\frac{\partial}{\partial x_k}\left[\rho\overline{u_i'u_j'u_k'}+\overline{p\left(\delta_{kj}u_i'+\delta_{ik}u_j'\right)}\right]}_{D_{T,ij}=\text{Turblent diffusion}}+\underbrace{\frac{\partial}{\partial x_k}\left[\mu\frac{\partial}{\partial x_k}\left(\overline{u_i'u_j'}\right)\right]}_{D_{L,ij}=\text{Molecular diffusion}}$$

$$\underbrace{-\rho\left(\overline{u_i'u_k'}\frac{\partial u_j}{\partial x_k}+\overline{u_j'u_k'}\frac{\partial u_i}{\partial x_k}\right)}_{P_{ij}=\text{Stress production}}+\underbrace{\overline{\frac{p}{\rho}\left(\frac{\partial u_i'}{\partial x_j}+\frac{\partial u_j'}{\partial x_i}\right)}}_{\phi_{ij}=\text{Pressure strain}}\underbrace{-2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}}_{\varepsilon_{ij}=\text{Dissipation}}$$

$$\underbrace{-2\rho\Omega_k\left(\overline{u_j'u_m'}\varepsilon_{ikm}+\overline{u_i'u_m'}\varepsilon_{jkm}\right)}_{F_{ij}=\text{Production by system rotation}} \qquad (3\text{-}11)$$

The Ω_k is an angular velocity and both ε_{ikm} and ε_{jkm} are permutation tensors. Of the various terms in these exact equations, C_{ij}, $D_{L,ij}$, P_{ij}, and F_{ij} do not require any modelling. However, $D_{T,ij}$, ϕ_{ij}, and ε_{ij} need to be modelled to close the equations. The reason is simply because the averaging procedure of $\overline{u_i'u_j'u_k'}$ will generate a lot of unknown variables and it becomes impossible to solve them directly. The turbulent diffusivity transport term is modelled using a simplified form of the generalised gradient diffusion hypothesis as:

$$D_{T,ij}=\frac{\partial}{\partial x_k}\left[\frac{\mu_t}{\sigma_k}\frac{\partial\left(\overline{u_i'u_j'}\right)}{\partial x_k}\right] \qquad (3\text{-}12)$$

The pressure strain term is modelled as:

$$\phi_{ij}=\overline{\frac{p}{\rho}\left(\frac{\partial u_i'}{\partial x_j}+\frac{\partial u_j'}{\partial x_i}\right)}=-C_1\frac{\varepsilon}{k}\left[\overline{u_i'u_j'}-\frac{2}{3}\delta_{ij}k\right]-C_2\left[P_{ij}-\frac{2}{3}\delta_{ij}P\right] \qquad (3\text{-}13)$$

where $P = 0.5P_{ij}$ is the turbulence production due to shear, and the constants are C_1 = 1.8 and C_2 = 0.6.

The dissipation term is assumed to be isotropic and is approximated by:

$$\varepsilon_{ij} = 2\mu \overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}} = \frac{2}{3}\delta_{ij}\varepsilon \tag{3-14}$$

The scalar dissipation rate is computed with a model transport equation similar to the one in the standard *k*-*ε* model.

The LES model assumes that the large eddies of the flow are dependent on the flow geometry and boundary conditions, while the smaller eddies are self-similar and have a universal character. Thus, in LES the large unsteady vortices are solved directly by the filtered Navier-Stokes equations, while the effect of the smaller universal scales (sub-grid scales) are modelled using a sub-grid scale (SGS) model. A filtered Navier-Stokes equation is given by:

$$\frac{\partial}{\partial t}(\rho \bar{u}_i) + \frac{\partial}{\partial x_j}(\rho \bar{u}_i \bar{u}_j) = \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \sigma_{ij}}{\partial x_j}\right) - \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial \bar{p}}{\partial x_i} \tag{3-15}$$

where σ_{ij} is the stress tensor due to molecular viscosity given by:

$$\sigma_{ij} = \left[v\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right] - \frac{2}{3}\mu \frac{\partial \bar{u}_l}{\partial \bar{x}_l}\delta_{ij} \tag{3-16}$$

and τ_{ij} is the SGS stress given by:

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\mu_t \bar{S}_{ij} \tag{3-17}$$

The μ_t is the SGS turbulent viscosity, and $\bar{S}_{ij}$, is rate-of-strain tensor for the resolved scale defined by:

$$\bar{S}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \tag{3-18}$$

The overbar from eq.(3-15) to eq.(3-19) denotes a resolved scale quantity rather than a time-averaged. The most commonly used SGS model is the Smagorinsky (1963) model, which has been further developed by Lilly (1966). They compensate for the unresolved turbulent scales through the addition of an isotropic turbulent viscosity into the governing equations. In the Smagorinsky-Lilly model the turbulent viscosity is modelled by:

$$\mu_t = \rho L_s^2 \left|\bar{S}\right| \tag{3-19}$$

where L_s is the mixing length for sub-grid scales and $\left|\bar{S}\right| = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$. L_s can be calculated from:

$$L_s = \min\left(\kappa d, C_s V^{1/3}\right) \tag{3-20}$$

where κ = 0.42, d is the distance to the closest wall, C_s = 0.1 is the Smagorinsky constant, and V is the volume of the computational cell. A LES was performed in this work to evaluate the effect of unresolved eddies near the impeller wall and hence on the turbulence and mean velocities predictions. It has to be noted that the y^+ around the impeller wall in this work ranging from 5 to 40 which is not optimal for LES. To our best of knowledge, the effect of the unresolved eddies near the impeller wall to the LES prediction has not been evaluated comprehensively for a stirred tank flow, especially when dealing with angle-resolved flow quantities.

DES as mentioned earlier belongs to a class of a hybrid turbulence models which blend LES away from boundary layer and RANS near the wall. This model was introduced by Spalart *et al.* (1997) in an effort to reduce the overall computational effort of LES modelling by allowing a coarser grid within the boundary layers. The DES employed for the turbulence modelling in this work is based on the Spalart-Allmaras (SA) model (Fluent 6.2, 2005).

The SA one-equation model solves a single partial differential equation for a variable $\tilde{\nu}$ which is related to the turbulent viscosity. The variable $\tilde{\nu}$ is identical to the turbulent kinematic viscosity except in the near-wall (viscous-affected) region. The model includes a wall destruction term that reduces the turbulent viscosity in the log layer and laminar sub-layer. The transport equation for DES is:

$$\frac{\partial}{\partial t}(\rho\tilde{\nu})+\frac{\partial}{\partial x_i}(\rho\tilde{\nu}u_i)=G_v+\frac{1}{\sigma_{\tilde{\nu}}}\left[\frac{\partial}{\partial x_j}\left\{(\mu+\rho\tilde{\nu})\frac{\partial\tilde{\nu}}{\partial x_j}\right\}+C_{b2}\rho\left(\frac{\partial\tilde{\nu}}{\partial x_j}\right)^2\right]-Y_v \tag{3-21}$$

The turbulent viscosity is determined via:

$$\mu_t=\rho\tilde{\nu}f_{v1},\quad f_{v1}=\frac{\chi^3}{\chi^3+C_{v1}^3},\quad \chi\equiv\frac{\tilde{\nu}}{\nu} \tag{3-22}$$

where $\nu = \mu/\rho$ is the molecular kinematic viscosity. The production term, G_v, is modelled as:

$$G_v=C_{b1}\rho\tilde{S}\tilde{\nu},\quad \tilde{S}\equiv S+\frac{\tilde{\nu}}{k^2d^2}f_{v2},\quad f_{v2}=1-\frac{\chi}{1+\chi f_{v1}} \tag{3-23}$$

S is a scalar measure of the deformation rate tensor which is based on the vorticity magnitude in the SA model. The destruction term is modelled as:

$$Y_v=C_{w1}\rho f_w\left(\frac{\tilde{\nu}}{d}\right)^2,\quad f_w=g\left[\frac{1+C_{w3}^6}{g^6+C_{w3}^6}\right]^{1/6},\quad g=r+C_{w2}\left(r^6-r\right),\quad r\equiv\frac{\tilde{\nu}}{\tilde{S}k^2d^2} \tag{3-24}$$

The closure coefficients for SA model (Spalart and allmaras, 1992) are $C_{b1} = 0.1355$, $C_{b2} = 0.622$, $\sigma_{\tilde{v}} = \frac{2}{3}$, $C_{v1} = 7.1$, $C_{w1} = \frac{C_{b1}}{k^2} + \frac{(1 + C_{b2})}{\sigma_{\tilde{v}}}$, $C_{w2} = 0.3$, $C_{w3} = 2.0$, $k = 0.4187$.

In the SA model the destruction term (eq.3- 24) is proportional to $(\tilde{v}/d)^2$. When this term is balanced with the production term, the eddy viscosity becomes proportional to $\tilde{S}d^2$. The Smagorinsky LES model varies its sub-grid-scale (SGS) turbulent viscosity with the local strain rate, and the grid spacing is described by $v_{SGS}\ \alpha\ \tilde{S}\Delta^2$ in eq.(3-19), where Δ = max(Δ*x*, Δ*y*, Δ*z*). If *d* is replaced with Δ in the wall destruction term, the SA model will act like a LES model. To exhibit both RANS and LES behaviour, *d* in the SA model is replaced by:

$$\tilde{d} = \min(d,\ C_{des}\Delta) \tag{3-25}$$

where C_{des} is a constant with a value of 0.65. Then the distance to the closest wall *d* in the SA model is replaced with the new length scale $\tilde{d}$ to obtain the DES. The purpose of using this new length is that in boundary layers where Δ far exceeds *d*, then the standard SA model applies since $\tilde{d} = d$. Away from walls where $\tilde{d} = C_{des}\Delta$, the model turns into a simple one equation SGS model, close to Smagorinsky's in the sense that both make the mixing length proportional to Δ. The Smagorinsky model is the standard eddy viscosity model for LES. On the other hand, this approach retains the full sensitivity of RANS model predictions in the boundary layer. This model has never been applied to predict the spray drying flows in the past and so this is an objective of the current study.

3.5.2 Particle Heat and Mass transfer

The species transport model was selected with DPM to enable the prediction of simultaneous heat and mass transfer during the drying process. The combined

Eulerian and Lagrangian model is used to obtain particle trajectories by solving the force balance equation:

$$\frac{d\underline{u}_p}{dt} = \frac{18\mu}{\rho_p {d_p}^2}\frac{C_D Re}{24}\left(\underline{v} - \underline{u}_p\right) + \underline{g}\left[\frac{\rho_p - \rho_g}{\rho_p}\right] \tag{3-26}$$

Where $\underline{v}$ is the fluid phase velocity, $\underline{u}_p$ is the particle velocity, ρ_g is the density of fluid and ρ_p is the density of the particle.

The particle force balance includes discrete inertia, aerodynamic drag and gravity. The slip Reynolds number (Re) and drag coefficient (C_D) are given in the following equations.

$$Re = \frac{\rho_g d_p \left|\underline{u}_p - \underline{v}\right|}{\mu} \tag{3-27}$$

$$C_D = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} \tag{3-28}$$

Where, d_p is the particle diameter, and a_1, a_2, and a_3 are constants that apply to smooth spherical particles over several ranges of Re by Morsi and Alexander (1972).

The velocity of particle relative to air velocity was used in the trajectory calculation. Turbulent particle dispersion was included in this model as discrete eddy concept. In this approach, the turbulent air flow pattern is assumed to make up of a collection of randomly directed eddies, each with its own lifetime and size. Particles are injected into the flow domain at the nozzle point and envisaged to pass through these random eddies until they impact the wall or leave the flow domain through the product outlet. In this study, the particle stickiness and particle collisions (agglomeration) were not considered.

The heat and mass transfer between the particles and the hot gas is derived following the motion of the particles.

$$m_p c_p \frac{dT_p}{dt} = hA_p\left(T_g - T_P\right) + \frac{dm_p}{dt} h_{fg} \quad (3\text{-}29)$$

Where m_p is the mass of the particle, C_p is the particle specific heat, T_p is the particle temperature, h_{fg} is the latent heat A_p is the surface area of the particle and h is the heat transfer co-efficient.

The mass transfer rate between the gas and particles is calculated from the following equation.

$$\frac{dm_p}{dt} = -k_c A_p\left({Y_s}^* - Y_g\right) \quad (3\text{-}30)$$

Where Y_s* is the saturation humidity, Y_g is the gas humidity and k_c is the mass transfer coefficient.

3.5.3 Computational grid

Anandharamakrishnan *et al.* (2007), who had been studied on particle history during spray dryer CFD simulations indicates that a three-dimensional (3D) model is more suitable for analyzing a spray drying system rather than two-dimensional (2D) model studied by Kieviet (1997). The 2D model does not give the actual primary particle residence time as total recirculation zone was not considered. In CFD approach, the computational grid has a significant effect on the simulation accuracy, as well as the computational effort needed to solve the entire problems. Research by

Mezhericher *et al.* (2009) in modelling of droplet drying in spray chambers using two-dimension and three-dimension CFD had found that, 2D axi-symmetric model is suitable for fast and low resource consumption numerical calculations and it can predict the value of velocity, temperature, and vapor fraction in the spray chamber accurately. However, due to restrictions, 2D model fails to predict asymmetry of flow patterns and presence of the transversal air flow. This model also cannot provide an actual 3D picture of particle trajectories inside the spray chamber. The researcher highlighted, in the case when the above characteristics are important, the utilization of 3D model is essential. Therefore, in this work, the 3D model had been implementing in order to get accuracy prediction.

3.6 Summary

The review presented in this chapter clearly shows that, there still many unsolved issues on spray drying modelling especially related to the accurate prediction of *k*, ε, and axial velocity of turbulent flow especially in complex spray dryer geometric. There are very a few studied have attempted to predict the turbulent flow detail close to the wall. It is possible to overcome such issues by applying the new invented turbulence model, DES, which has a great potential of resolving the turbulent flow. But it needs to be validated before it can be applied further for another spray drying modelling.

CHAPTER 4

4.0 RESULTS AND DISCUSSIONS

4.1 Overview

In this chapter 4, mainly presents the DES and RANS calculations on the single phase turbulent flow in Case A: counter-current spray dryer tower; and the DES and standard k-ε (SKE) calculation on the single and multiphase flow in Case B: co-current spray dryer include the prediction of gas temperature and gas humidity with present of spray injection. The grid dependent for both case study also have presented. All the simulation prediction for both case studies have been evaluated and compared with available experimental data from the literature. This study confirmed the strength and weakness for every turbulence model used in this study.

4.2 Case A: Counter-current spray dryer tower

In this work, the prediction from the CFD simulation of single phase gas flow was compared to the Laser Doppler Anemometer (LDA) measurement by Bayly *et al.* (2004) at various positions of the spray drying chamber. Prediction data from CFD simulations were taken as a statistical average from up to 1000 time step after the pseudo convergence was achieved, which mimic the data collection in experimental measurement.

4.2.1 Grid dependent

The grid generation within computational region, play an important role in the prediction accuracy (Lin *et al.*, 1996). The grid generated as the control volume, which called as cell. Earlier, Bayly *et al.* (2004) about employed 503k grid to yield a satisfactory prediction using the RSM turbulence model. Nevertheless, the grid dependent study was performed to confirm the suitability of the prepared grid. As it shown in Figure 4-2, there are minimal differences between the predictions obtained using both the 503k and 934k grid. Thus, the 503k grid was used for the remaining of this work in interest to minimize the computational time.

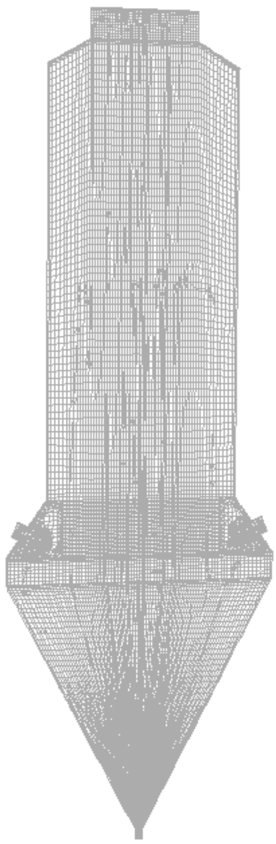
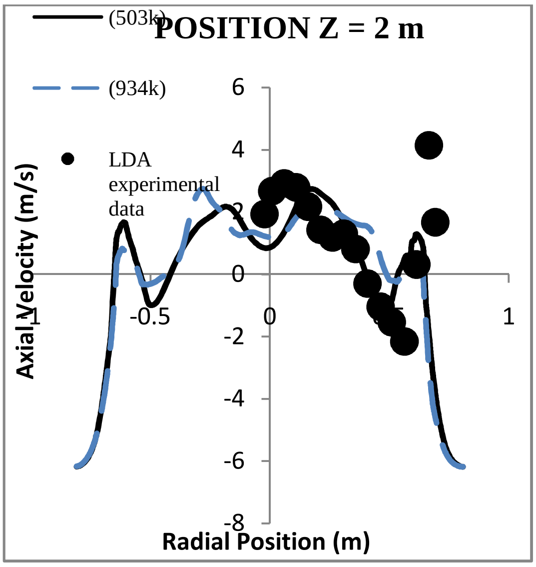


Figure 4-1: Grid used in the counter-current spray dryer simulation



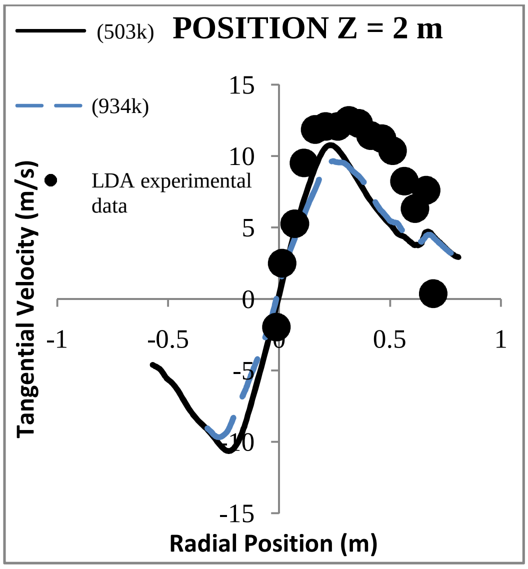


Figure 4-2: Result from grid dependent study

4.2.2 Prediction of gas flow velocity in counter-current spray dryer

The axial positions for comparison of measurements and simulation of gas flow velocity in counter-current spray dryer are shown in Figure 4-3. Generally, all CFD models tested in this work can predict the flow pattern in counter-current spray drying reasonably. However, ultimate agreement was not achieved. Prediction by the DES model is by far the best among the model tested. This is attributed by the fact that DES employs LES in the bulk flow which in turn provides much better predictions of the turbulence flow. Around the boundary layer (i.e. the wall) the DES turn to a single equation Spalart-Allmaras turbulence model which provides a fair approximation of the flow near the wall without necessarily having to resolve the small eddies. This method of hybrid LES-RANS model employed in DES reduces the overall computational demand of a full LES solution while at the same time maintaining the prediction accuracy.

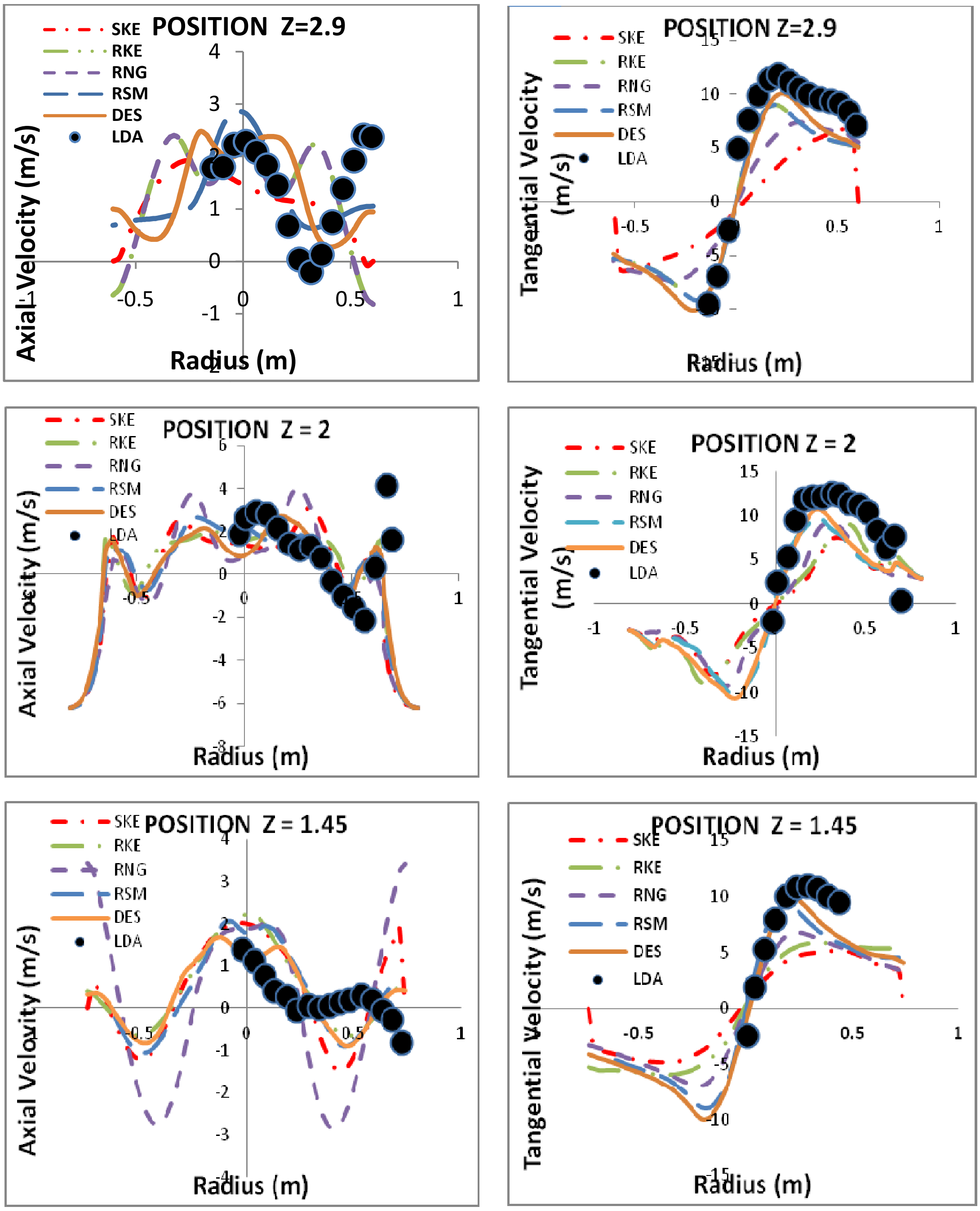


Figure 4-3: Prediction of axial and tangential velocity inside the counter-current spray dryer chamber using various turbulence models. Data points adopted from Bayly *et al.* (2004).

The RSM model outperformed all the other RANS based turbulence models (SKE, RKE and RNG) tested in this work. This is attributed by the anisotropic eddy viscosity model in RSM model, which is known for its excellent prediction for swirling and strong anisotropic turbulence flow such as in cyclone (Gimbun *et al.*, 2005; Slack *et al.*, 2000). As it is mentioned in the previous section, the flow pattern inside the counter-current spray dryer studied in this work exhibit some swirling flow due to the position and design of the inlet gas around the tower hip, hence requiring a more complicated turbulence model for accurate prediction of the mean flow field inside the chamber.

The RNG model also predicts the tangential velocity fairly well, marginally better than the other two equations turbulence model of SKE and RKE. This is due to the inclusion of the swirl term in RNG model, which was not included in the SKE and RKE models. However, predictions obtained from these two-equation turbulence models which assume isotropic eddy viscosity were generally poor in comparison to either DES or RSM.

The axial flow pattern exhibit a single peak pattern similar to those normally seen for a reverse flow cyclone (e.g. Fraser *et al.*, 2000). Again all models predict the axial flow pattern reasonably well compared to the experimental measurement. The DES and RSM models again provide much closer agreement to the experimental data in similar to the trend seen for the prediction of tangential velocity. Predictions by both RKE and RNG on the axial velocity are acceptable as the predicted value was relatively close to the experimental measurement. However, both RNG and RKE models may not be the best model for predicting the mean flow insider the counter-current spray dryer because they can produce somewhat unrealistic (triple peak) predictions on occasion (see Fig. 2 at Z = 2.9 m). The SKE model was the worst among all the turbulence models tested, and hence should be avoided for modelling of a counter-current spray dryer.

The multiphase model cannot be performed for the counter-current spray dryer due to limited data available from the literature.

4.3 Case B: Co-current spray dryer

In this work, the prediction from the CFD simulation of the flow pattern without (single phase) and with present of spray injection (multiphase) were compared with Kieviet (1997) experimental data at various positions of the spray drying chamber. Prediction data from CFD simulations were taken as a statistical average from up to 1000 time step after the pseudo convergence was achieved, which mimic the data collection in experimental measurement.

4.3.1 Grid dependent

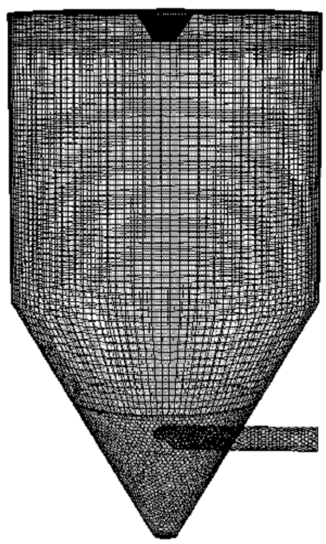


Figure 4-4: Grid used in the co-current spray dryer simulation

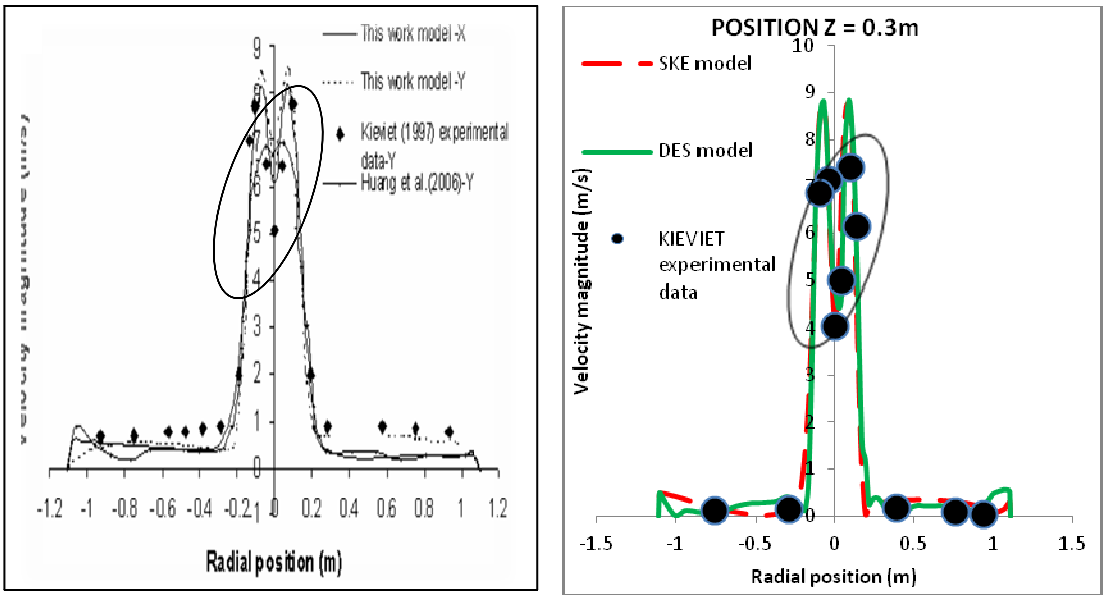


Figure 4-5: Comparison of the current simulation prediction with previous simulation prediction by Anandharamakrishnan *et al.* (2007) and Huang *et al.* (2006)

Figure 4-5, shown the better prediction of the air velocity magnitude and in good agreement with the data pointed adopted from kieviet (1997). CFD prediction in this work is also much better compared to the previous research by Anandharamakrishnan *et al.* (2007) and Huang *et al.* (2006). This is due to the fact that grid used in this work is finer than the one used by Anandharamakrishnan *et al.* (2007). The current simulation performed using about 450k grid cells, whereas the grid produced by Anandharamakrishnan (2007) consist only about 295k cells and Huang *et al.* (2006) did not mention their grid number explicitly, however it is suspected to be much lower than the one by Anandharamakrishnan *et al.* (2007) seeing from the lower accuracy of their prediction.

4.3.2 Prediction of gas flow velocity profile in co-current spray dryer without spray injection

The gas flow velocity in co-current spray dryer for comparison of measurements and simulation are shown in Figure 4-6.

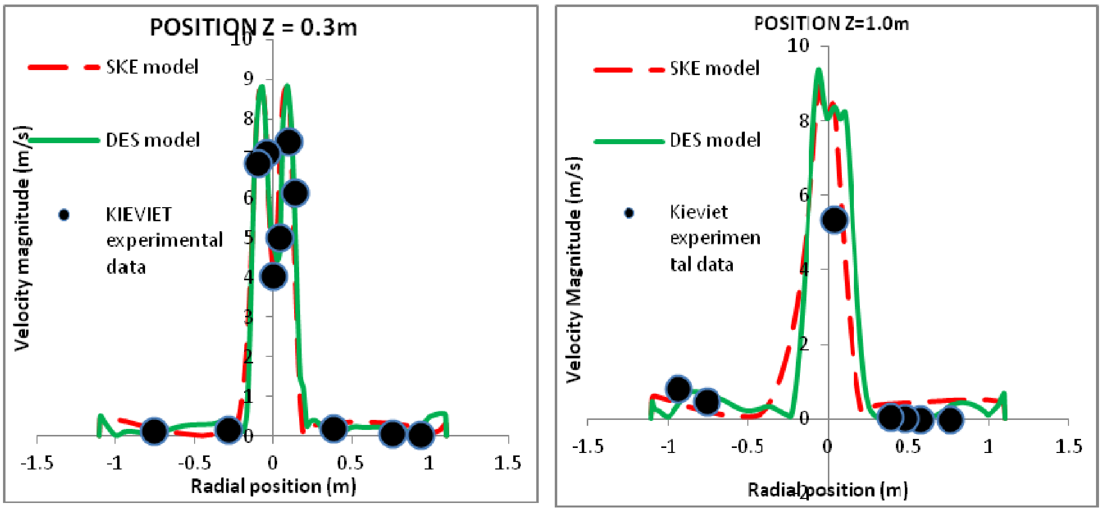


Figure 4-6: Prediction of gas velocity magnitude inside the co-current spray dryer chamber using standard *k*-*ε* and DES models. Data points adopted from Kieviet, (1997).

The gas velocity magnitude profile are plotted at two different positions (Z = 0.3 m and Z = 1.0 m from the top of co-current spray drying) as in Figure 4-6. The simulation prediction of two turbulence models (standard *k*-*ε* and DES models) data were compared with Kieviet (1997) experimental data.

The current simulation prediction by DES model had shown well agreement with Kieviet's (1997) experimental data as well as the SKE model. This is attributed to the fact that the DES employs the LES model in the bulk flow which in turn provides much better prediction of complex turbulence flow in co-current spray dryer. The DES turns to a single equation Spalart-Allamaras turbulence model which provides a fair approximation of the flow near boundary layer (i.e. the wall) without necessarily having to resolve the small eddies. Same as mention before, this method of hybrid LES-RANS model employed in DES reduces the overall computational demand of a full LES solution while at the same time maintaining the prediction accuracy.

The SKE model is commonly used because it converges considerably faster than other RANS model. The SKE model can predicts the mean velocity as good as the DES model in this case because the co-current spray dryer do not feature a swirling flow pattern which would demand an extensive model such as RSM. Previous research by Anandharamakrishnan (2007) also use the SKE model, whereas Huang *et al.* (2006) used RNG turbulence model, and both work shows satisfactory agreement with Kieviet (1997) experimental data as it shown in Figure 4-5. The use of unsteady RANS in this work may also contribute to the good prediction compare to steady RANS by Anandharamakrishnan *et al.* (2007) and Huang *et al.* (2006). Unsteady RANS provides better prediction than steady RANS (Squires *et al.*, 2005).

4.3.2 Prediction of gas temperature profile with spray injection

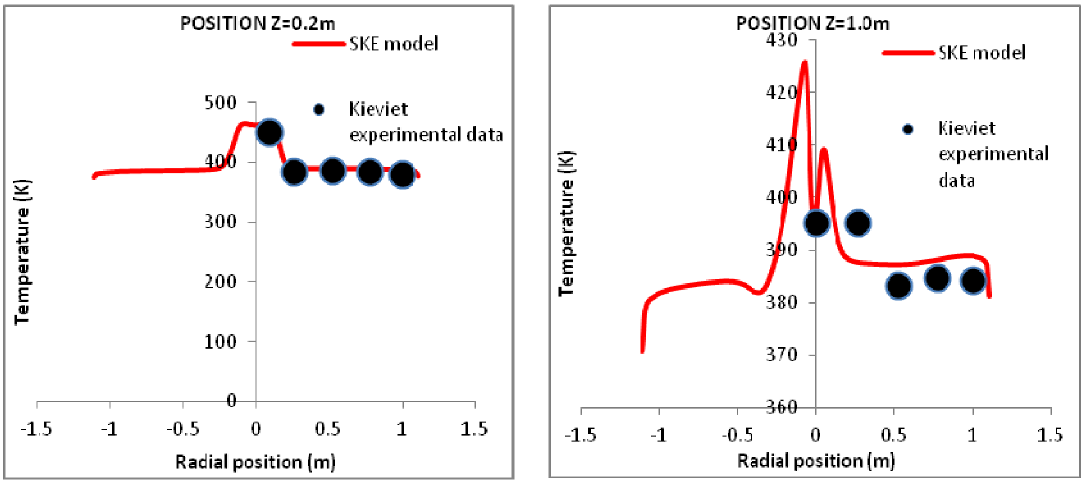


Figure 4-7: Prediction of gas temperature profile in co-current spray dryer chamber using standard k-ε. Data points adopted from Kieviet (1997).

Figure 4-7, shows the prediction of gas temperature with spray injection of Maltodextrin solution (multiphase flow) consists of 57.5% of water content. The simulation prediction at position Z = 0.2 m and z = 1.0 m from the top of co-current spray dryer chamber was compared with Kieviet's (1997) experimental data. The predictions were in good agreement with Kieviet's (1997) experimental data. The temperature prediction at position Z = 0.2 m was high due to the air inlet temperature about 468K. The gas temperature was decrease as the gas flow down to the bottom of the co-current spray dryer chamber as shown in positions Z = 1.0 m.

Figure 4-8, shown the simulation prediction of gas humidity profile in co-current spray dryer which is seem good prediction with the Kieviet's (1997) experimental data. The gas humidity presented as the water vapour mass fraction. The humidity profiles were similar in form to the gas temperature profile, but inverted due to simultaneous heat and mass transfer (Anandharamakrishnan, 2007).

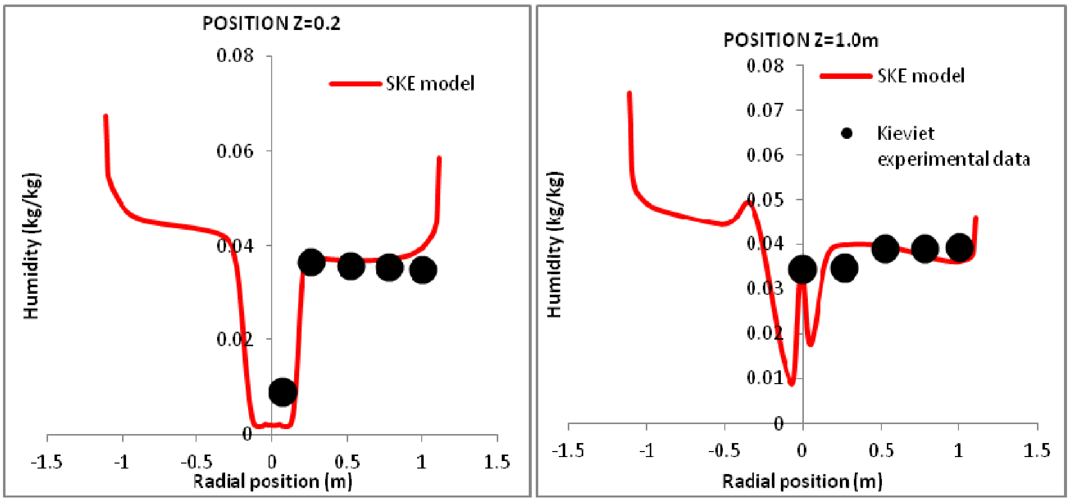


Figure 4-8: Prediction of gas humidity profile inside the co-current spray dryer chamber using standard *k*-*ε*. Data points adopted from Kieviet (1997).

However, only the SKE model can be employed to predict the gas temperature and gas humidity profile inside the co-current spray dryer. The reason is that, RANS have abilities to resolve prediction simply based on two-transport equation model solving for the turbulent kinetic energy (k) and its dissipation rate (ε) for single and multiphase prediction. The DES model which the hybrid of LES and RANS model, cannot be calculate in multiphase prediction due to the weakness of LES model (Fluent 6.3, 2006).

4.4 Summary

CFD simulation of counter-current and co-current spray dryer have been developed and the predictions obtained using various turbulence model has uncovered a great potential of DES for modelling the flow field of counter-current and co-current spray dryer. However the DES model cannot be use to predict particle tracking purpose in multiphase flow study due to the weakness of LES model employed by DES turbulence model.

The number of grid for both cases also affects the accuracy of the CFD prediction. More accurate prediction was observed when the total number of grid cell increased. It is also note worthy to consider employing the unsteady solver for predicting the hydrodynamics in spray dryer as it gives much accurate prediction.

CHAPTER 5

5.0 CONCLUSION AND RECOMMENDATION

5.1 Conclusions

In this study, computational methods have been applied to investigate the fluid mechanics of single phase and multiphase in two common types of spray drying (counter-current and co-current spray dryer). Most of the work deals with CFD simulation. The aim of this study is to develop a modelling method for hydrodynamics for predicting air flow pattern in spray dryer chamber to make possible the modelling spray drying via CFD.

CFD simulation of counter-current and co-current spray dryer have been developed and the predictions obtained using various turbulence model has uncovered a great potential of DES for modelling the flow field of counter-current and co-current spray dryer. However the DES model cannot be use to predict particle tracking purpose in multiphase flow study due to the weakness of LES model employed by DES turbulence model.

The number of grid for both cases also affects the accuracy of the CFD prediction. More accurate prediction was observed when the total number of grid cell increased. It is also note worthy to consider employing the unsteady solver for predicting the hydrodynamics in spray dryer as it gives much accurate prediction. Results from this simulation may be useful for development of a more comprehensive and accurate model for counter-current and co-current spray dryer in the future.

5.2 Recommendation

From this study, it was found that, the DES model cannot be used to predict fluid particle interaction. Therefore the DES model needs further development in order to perform the particle tracking in CFD simulation, and hence can be applied to do spray drying simulation.

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APPENDIX A

Thu, March 25, 2010 4:24:56 PM

[SOMCHE2010 / ICPEAM2010] Your paper #1569285107

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To: Jolius Gimbun <jolius@ump.edu.my>

Cc: Siti Ferdaus Aspari <siti_ferdaus@yahoo.com>; laukokkeong@petronas.com.my

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NOTIFICATION OF ACCEPTANCE

Invitation to International Conference on Process Engineering and Advanced Material (ICPEAM2010)/ 24th Symposium of Malaysian Chemical Engineers (SOMChE2010), 15th-17th June 2010, Kuala Lumpur Convention Centre, Kuala Lumpur, Malaysia.

Reference (Paper Code): 1569285107

Paper Title: "CFD Simulation of Hydrodynamics in Counter-Current Spray Dryer Tower"

Dear Dr. Jolius Gimbun,

It is our great pleasure to inform you that your paper has been accepted for ORAL presentation in the International Conference on Process Engineering and Advanced Material (ICPEAM2010)/ 24th Symposium of Malaysian Chemical Engineers(SOMChE2010).

On behalf of the organising committee, I would like to invite you to participate in this conference.

Listed below are the reviews for your paper. You are required to revise your paper based on the comment recommended by the reviewer. The reviews below can be found at http://edas.info/showPaper.php?m=1569285107 using your EDAS username jolius@ump.edu.my.

You should submit the final version of your paper in WORD format (.doc) latest by 30th April 2010.

According to the conference policy, only papers with confirmed payment will be included in the conference proceeding.

Registration and payment are required to be conducted through EDAS. The registration and payment system will be activated starting from 19th March 2010 and closed by 1st June 2010. Kindly refer to our website (under the Registration Section) for the procedures of registration and payment through EDAS: http://www.utp.edu.my/icpeam2010/index.php?option=com_content&view=article&id=48&Itemid=14

Early Registration: By 30th April 2010 (10% discount on registration fee)

Late Registration: After 30th April 2010

You may obtain additional information for traveling and accommodation from our

website:
http://www.utp.edu.my/estcon2010/index.php?option=com_content&view=article&id=48&Itemid=37

We look forward to seeing you in Kuala Lumpur.

Yours sincerely,

Dr Shuhaimi Mahadzir

Chair of Organising Committee

ICPEAM2010/SOMChE2010

======= Review 1 ======

> *** Comments to Authors: Please highlight to the authors the strengths and weaknesses of their paper and justify your assessment. Please indicate any changes that should be made to the paper if it is accepted.

strength
very focus work on CFD simulation. the explanation was direct to the point and brief.
perhaps, for journal publication, the contents need to be expanded.

weakness
probably because the content is small, the paper looks simple. but, sufficient as a conference paper.

> *** Relevance and Timeliness: Please rate the relevance of the paper to the

conference, and the importance of the topic addressed in the paper and its timeliness within its area of research.

Average (3)

> *** Novelty and Originality: Please rate the novelty and originality of the work presented in the paper

Average (3)

> *** Technical Content and Correctness: Please rate the technical contents of the paper, its soundness and scientific rigour

Average (3)

> *** Quality of Presentation: Please rate the quality of presentation including (i)paper organization, (ii)clearness of text and figures,(iii)completeness and accuracy of references, and (iv)correct usage of English

Average (3)

> *** Overall Recommendation: Please indicate your overall recommendation Accept (4)

======= Review 2 =======

> *** Comments to Authors: Please highlight to the authors the strengths and weaknesses of their paper and justify your assessment. Please indicate any changes that should be made to the paper if it is accepted.

please use official email

show grid independence in Fig2

try to convert all the mesh as hexa

Try SST or V2F models for better results

redraw the plots in fig2 in sigmaplot or tecplot (to improve the quality)

> *** Relevance and Timeliness: Please rate the relevance of the paper to the conference, and the importance of the topic addressed in the paper and its timeliness within its area of research.

Average (3)

> *** Novelty and Originality: Please rate the novelty and originality of the work presented in the paper

Average (3)

> *** Technical Content and Correctness: Please rate the technical contents of the paper, its soundness and scientific rigour

Average (3)

> *** Quality of Presentation: Please rate the quality of presentation including (i)paper organization, (ii)clearness of text and figures,(iii)completeness and accuracy of references, and (iv)correct usage of English

Average (3)

> *** Overall Recommendation: Please indicate your overall recommendation Accept (4)

CFD Simulation of Hydrodynamics in Counter-Current Spray Dryer Tower

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***Abstract*-This paper presents Computational fluid dynamics (CFD) modelling of hydrodynamics in a counter current spray drying tower. The simulations were performed using five different turbulent models, i.e. standard k-ε, RNG k-ε, Realizable k-ε, Reynolds stress models and the Detached Eddy Simulation. The predicted airflow patterns inside the spray drying chamber were found to be in fair agreement to the experimental data adopted from literature for all turbulence models tested in this work. A great potential of the Detached Eddy Simulation for predicting the flow pattern in a counter-current spray dryer was uncovered as its provides more accurate predictions compared to other models tested in this work.**

I. INTRODUCTION

Spray dryer is a well established method for converting liquid feed materials into dry powder forms. Spray dryer is widely used to produce foods such as whey, instant drinks, milk, tea and soups, as well as healthcare and pharmaceutical products, such as vitamins, enzymes and bacteria [1] also in production of fertilizers, detergent soap, and dyestuffs.

There is much research done on spray drying either by experimental or by using modelling reported in the literature such as Kieviet et al. [2], Anandharamakrishnan et al. [3], Southwell and Langrish [4], Harvie et al. [5] and Huang et al. [6]. Most of the previous work deals with a common co-current flow spray drying. Although simulation of the tall counter-current spray dryer was reported by Harvie et al. [5], but there are limited comparison made on the flow pattern inside the drying chamber. Bayly et al. [7] reported an extensive comparison between the experimental measurement and CFD simulation of a counter-current spray drying. The turbulence modelling was realised using a Reynolds Stress Models (RSM) model in their work, and it seems to give a good prediction of the swirling flow inside the drying chamber. However, there is a still discrepancy, especially on the prediction of gas axial velocity. Therefore, this work attempt to evaluate the performance of various turbulence models namely standard *k-ε* (SKE), RNG *k-ε* (RNG), Realizable *k-ε* (RKE), RSM and Detached Eddy Simulation (DES) for predicting the flow pattern in a counter-current spray dryer. The DES is a relatively new development in turbulence modelling, which is belonged to a hybrid turbulence model, which blend Large Eddy Simulation (LES) away from the boundary layer and RANS near the wall. This model was introduced by Sparlat et al. [8] in an effort to reduce the overall computational effort of LES modelling by allowing a coarser grid within the boundary layers. The DES employed for the turbulence modelling in this work is based on Spalart-Allmaras model and has never been previously used for modelling of spray drying.

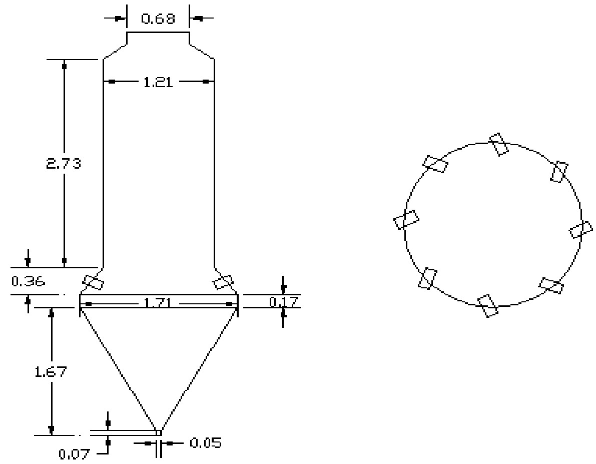

Figure 1. Spray-dryer geometry (right) and the main inlet position (left)

II. COMPUTATIONAL APPROACH

The commercial CFD code, FLUENT 6.3, was used to simulate the three-dimensional configuration of a counter-current tower spray dryer fitted with eight main inlets set around the tower hip. The main inlet cylinder shape was set 25° below the horizontal and 25° to the tower radius in the horizontal plane which imparting a significant swirl to the flow in the tower. GAMBIT was used to draw the spray dryer tower diagram illustrated in Fig. 1, which has the same dimension to the one studied by Bayly et al. [7]. The simulation was performed using counter-current spray drying tower composed mainly consisting of about (503K) hexahedral and tetrahedral cells. Earlier, Bayly et al. [7] employed 500k grid to yield a satisfactory prediction using the RSM turbulence model. Nevertheless, the grid dependent study was performed to confirm the suitability of the prepared grid. As it shown in Fig. 2, there are minimal differences between the prediction obtained using both the 503k and 934k grid. Thus, the 503k grid was used for the remaining of this work in interest to minimise the computational time.

The total air flow through the eight main inlets to the tower is 3814 m^3/hr and for the based inlet airflow is 239 m^3/hr. The SIMPLE method was used for the pressure-velocity coupling and the 2nd order differencing for momentum terms for the RANS modelling, whereas the bounded central differencing was used for the DES simulation. Five different turbulence models namely the SKE, RNG, RKE, RSM and DES were employed in the simulation.

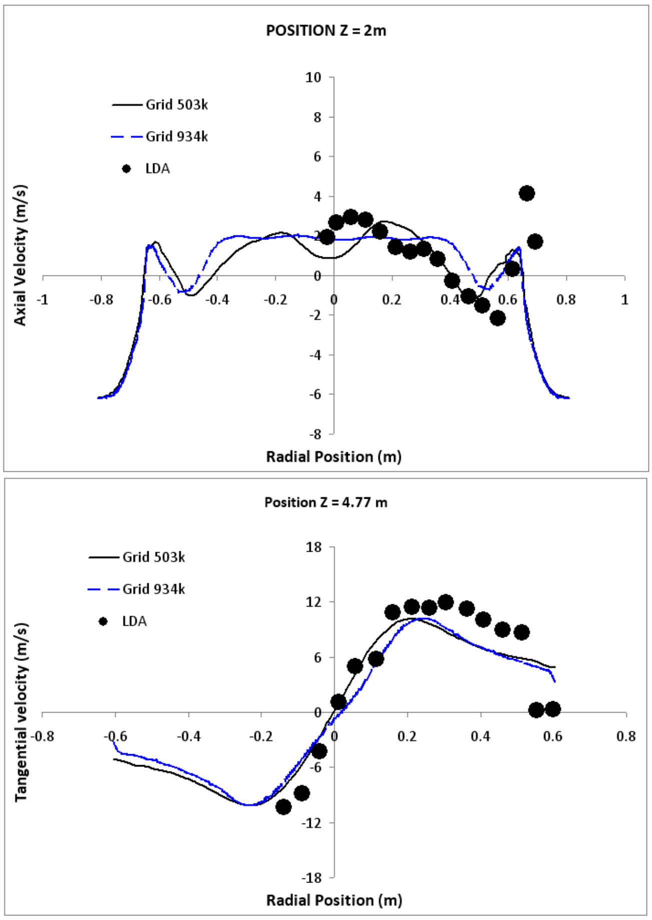

Figure 2: Result from grid dependent study

The standard *k-ε* model is a semi-empirical model based on transport equations for the turbulent kinetic energy and its dissipation rate. Transport equations for *k* and *ε* for all *k-ε* variant models can be generalised as follow:

$$\underbrace{\frac{\partial(\rho k)}{\partial t}}_{\text{timederivative}} + \underbrace{\frac{\partial}{\partial x_i}(\rho u_i k)}_{\text{convection}} = \underbrace{\frac{\partial}{\partial x_i}\left(\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right)}_{\text{diffusion}} + \underbrace{\rho P_k}_{\text{production}} - \underbrace{\rho\varepsilon}_{\text{destruction}} \qquad (1)$$

and

$$\underbrace{\frac{\partial(\rho\varepsilon)}{\partial t}}_{\text{time derivative}} + \underbrace{\frac{\partial}{\partial x_i}(\rho u_i \varepsilon)}_{\text{convection}} = \underbrace{\frac{\partial}{\partial x_i}\left(\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right)}_{\text{diffusion}} + \underbrace{S_\varepsilon}_{\text{source term}} \qquad (2)$$

The turbulent (eddy) viscosity, μ_t, is obtained from:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \qquad (3)$$

The relation for production term P_k, for the *k-ε* variant models (i.e. *k-ε*,*Rk-ε* and RNG) is given as:

$$P_k = \mu_t\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_j}{\partial x_i} \qquad (4)$$

For the standard *k-ε* model the source term, S_ε,is given by:

$$S_\varepsilon = \rho\left(C_{1\varepsilon}\frac{\varepsilon}{k}P_k - C_{2\varepsilon}\frac{\varepsilon^2}{k}\right) \qquad (5)$$

The model constants are [9] : $C_{\varepsilon 1}$ = 1.44, $C_{\varepsilon 2}$ = 1.92, C_μ = 0.09 σ_ε = 1.3 derived from correlation of experimental data.

This model widely used despite the known limitation of the model. The standard *k-ε* model perform was poorly for complex flows involving severe pressure gradient, separation and strong streamline curvature. Improvements have been made to the model to improve its predictive capability leading to an introduction of its variants, Realizable *k-ε* model, which was first introduced by Shih et al. [10]. The RKE model allows certain mathematical constraint to be obeyed which ultimately improves the performance of this model. RKE different from SKE model in two ways; first it has a new formulation of turbulent viscosity and second it is employs a new transport equation for this dissipation rate. RKE model still has similar equation from SKE model, except the C_μ is no longer constant, instead is a function of velocity gradients given as:

$$C_\mu = \frac{1}{A_o + A_s\dfrac{U^* k}{\varepsilon}} \qquad (6)$$

with A=4.04 $A_s = \sqrt{6}\cos\phi$ $\phi = \frac{\cos^{-1}(\sqrt{6}w)}{3}, w = \frac{S_{ij}S_{jk}S_{ki}}{\tilde{S}^3}$ $U^* = \sqrt{S_{ij}S_{ij} + \tilde{\Omega}_{ij}\tilde{\Omega}_{ij}}$ and $\tilde{S} = \sqrt{S_{ij}S_{ij}}$ to ensure positivity of normal stresses ($\overline{u_i^2} \geq 0$) and Schwarz's inequality for shear stress ($(\overline{u_i u_j})^2 \leq \overline{u_i^2}\,\overline{u_j^2}$). The Schwarz inequality for shear stresses in *k-ε* model can be violated when the mean strain rate is large, but it can be eliminated by having a variable C_μ[11].

The source term, S_ε for RKE is now given as:

$$S_\varepsilon = \rho\left(C_1 S\varepsilon - C_2\frac{\varepsilon^2}{k+\sqrt{\upsilon\varepsilon}}\right) \qquad (7)$$

The model constants are [10]: $C_1 = \max\left[0.43; \frac{\eta}{\eta+5}\right]$, $C_2 = 1.9$, $\sigma_k = 1$ and $\sigma_\varepsilon = 1.2$ with $\eta = Sk/\varepsilon$, and $S = \sqrt{2S_{ij}S_{ij}}$ is a modulus of mean rate of strain tensor.

RKE model offers largely the same benefits and has similar application as RNG. This RKE is a model possibly more accurate and easier to converge than RNG. However RNG have significant changes in the ε equation improves the ability to model highly strained flows. RNG model additional options aid in predicting swirling and flow Reynolds number flows.

The RNG model was obtained from renormalization group theory by Yakhot and Orzag [12]. RNG differs from standard *k-ε* because it has an additional term, *α*, in the *ε* transport equation, besides providing an analytical formula for the turbulent Prandtl numbers derived using RNG theory. Thus the source term S_ε for RNG is given by:

$$S_\varepsilon = \rho\left(C_{1,RNG}\frac{\varepsilon}{k}P_k - \sigma^{-1}\frac{\varepsilon^2}{k} - C_{2,RNG}\frac{\varepsilon^2}{k}\right) \qquad (8)$$

where σ^{-1} is the inverse effective Prandtl number given by

$$\sigma^{-1} = \frac{C_\mu \eta^3 (1-\eta/\eta_0)}{1+\beta\eta^3} \tag{9}$$

Instead of constant value for turbulent Prandtl number in *k*-ε, it is provided analytically in RNG by the following equation:

$$\left|\frac{\sigma^{-1}-1.3929}{\sigma_0^{-1}-1.3929}\right|^{0.6321}\left|\frac{\sigma^{-1}-2.3929}{\sigma_0^{-1}-2.3929}\right|^{0.3679} = \frac{\mu_{mol}}{\mu_{eff}} \tag{10}$$

where σ_0^{-1} = 1.0. In the high Reynolds number limit ($\mu_{mol}/\mu_{eff} << 1$), the inverse turbulent Prandtl number is $\sigma_k^{-1} = \sigma_\varepsilon^{-1} \approx 1.393$. Similar to the *Rk*-ε model, $\eta = Sk/\varepsilon$, and $S = \sqrt{2S_{ij}S_{ij}}$ is a modulus of mean rate of strain tensor, $\eta_0 = 4.38$, $\beta = 0.012$. The model constants are $C_{\varepsilon 1} = 1.42$, $C_{\varepsilon 2} = 1.68$, $\sigma_k = 1.393$, $\sigma_\varepsilon = 1.393$ derived from RNG theory by Yakhot and Orzag [12].

RSM abandons the assumption of the isotropic eddy-viscosity hypothesis, to close the Reynolds-averaged Navier-Stokes equations, by solving transport equations for the individual Reynolds stresses, together with a transport equation for the dissipation rate. RSM has a greater potential to give accurate predictions for complex flows, as it takes into accounts the effects of streamline curvature, swirl, rotation, and rapid changes in strain rate in a more rigorous manner than two-equation models such as *k*-ε. The foundation of RSM is the exact set of transport equations:

$$\underbrace{\frac{\partial}{\partial t}\left(\rho\overline{u_i'u_j'}\right)}_{\text{Time derivative}}+\underbrace{\frac{\partial}{\partial x_k}\left(\rho u_k\overline{u_i'u_j'}\right)}_{C_{ij}=\text{Convection}}=\underbrace{-\frac{\partial}{\partial x_k}\left[\rho\overline{u_i'u_j'u_k'}+\overline{p\left(\delta_{kj}u_i'+\delta_{ik}u_j'\right)}\right]}_{D_{T,ij}=\text{Turblent diffusion}}+$$

$$\underbrace{\frac{\partial}{\partial x_k}\left[\mu\frac{\partial}{\partial x_k}\left(\overline{u_i'u_j'}\right)\right]}_{D_{L,ij}=\text{Molecular diffusion}}\underbrace{-\rho\left(\overline{u_i'u_k'}\frac{\partial u_j}{\partial x_k}+\overline{u_j'u_k'}\frac{\partial u_i}{\partial x_k}\right)}_{P_{ij}=\text{Stress production}}+\underbrace{\overline{\frac{p}{\rho}\left(\frac{\partial u_i'}{\partial x_j}+\frac{\partial u_j'}{\partial x_i}\right)}}_{\phi_{ij}=\text{Pressure strain}}-$$

$$\underbrace{2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}}}_{\varepsilon_{ij}=\text{Dissipation}}\underbrace{-2\rho\Omega_k\left(\overline{u_j'u_m'}\varepsilon_{ikm}+\overline{u_i'u_m'}\varepsilon_{jkm}\right)}_{F_{ij}=\text{Production by system rotation}} \tag{11}$$

The Ω_k is an angular velocity and both ε_{ikm} and ε_{jkm} are permutation tensors. Of the various terms in these exact equations, C_{ij}, $D_{L,ij}$, P_{ij}, and F_{ij} do not require any modelling. However, $D_{T,ij}$, ϕ_{ij}, and ε_{ij} need to be modelled to close the equations. The reason is simply because the averaging procedure of $\overline{u_i'u_j'u_k'}$ will generate a lot of unknown variables and it becomes impossible to solve them directly.

The turbulent diffusivity transport term is modelled using a simplified form of the generalized gradient diffusion hypothesis as:

$$D_{T,ij} = \frac{\partial}{\partial x_k}\left[\frac{\mu_t}{\sigma_k}\frac{\partial\left(\overline{u_i'u_j'}\right)}{\partial x_k}\right] \tag{12}$$

The pressure strain term is modelled as:

$$\phi_{ij} = \overline{\frac{p}{\rho}\left(\frac{\partial u_i'}{\partial x_j}+\frac{\partial u_j'}{\partial x_i}\right)} = -C_1\frac{\varepsilon}{k}\left[\overline{u_i'u_j'}-\frac{2}{3}\delta_{ij}k\right]-C_2\left[P_{ij}-\frac{2}{3}\delta_{ij}P\right] \tag{13}$$

where $P=0.5P_{ij}$ is the turbulence production due to shear, and the constants are C_1=1.8 and C_2=0.6.

The dissipation term is assumed to be isotropic and is approximated by:

$$\varepsilon_{ij} = 2\mu\overline{\frac{\partial u_i'}{\partial x_k}\frac{\partial u_i'}{\partial x_k}} = \frac{2}{3}\delta_{ij}\varepsilon \tag{14}$$

The scalar dissipation rate is computed with a model transport equation similar to the one in the standard *k*-ε model.

DES model earlier belongs to a class of a hybrid turbulence models which blend LES away from boundary layer and RANS near the wall. This combination (RANS-LES) model was introduced by Spalart et al. [8] in an effort to reduce the overall computational of LES modelling by allowing the coarser grid at boundary layer. The DES employed for the turbulence modelling in this work is based on Spalart-Allmaras (SA) model [11] and has never been previously used for modelling of spray drying.

The SA one-equation model solves a single partial differential equation for a variable $\tilde{\nu}$ which is related to the turbulent viscosity. The variable $\tilde{\nu}$ is identical to the turbulent kinematic viscosity except in the near-wall (viscous-affected) region. The model includes a wall destruction term that reduces the turbulent viscosity in the log layer and laminar sub-layer. The transport equation for DES is:

$$\frac{\partial}{\partial t}(\rho\tilde{\nu})+\frac{\partial}{\partial x_i}(\rho\tilde{\nu}u_i)=G_\nu+\frac{1}{\sigma_{\tilde{\nu}}}\left[\frac{\partial}{\partial x_j}\left\{(\mu+\rho\tilde{\nu})\frac{\partial\tilde{\nu}}{\partial x_j}\right\}+C_{b2}\rho\left(\frac{\partial\tilde{\nu}}{\partial x_j}\right)^2\right]-Y_\nu \tag{15}$$

The turbulent viscosity is determined via:

$$\mu_t = \rho\tilde{\nu}f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3+C_{v1}^3}, \quad \chi \equiv \frac{\tilde{\nu}}{\nu} \tag{16}$$

where $\nu = \mu/\rho$ is the molecular kinematic viscosity. The production term, G_ν, is modelled as:

$$G_\nu = C_{b1}\rho\tilde{S}\tilde{\nu}, \quad \tilde{S} \equiv S+\frac{\tilde{\nu}}{k^2d^2}f_{v2}, \quad f_{v2} = 1-\frac{\chi}{1+\chi f_{v1}} \tag{17}$$

S is a scalar measure of the deformation rate tensor which is based on the vorticity magnitude in the SA model. The destruction term is modelled as:

$$Y_\nu = C_{w1}\rho f_w\left(\frac{\tilde{\nu}}{d}\right)^2, \quad f_w = g\left[\frac{1+C_{w3}^6}{g^6+C_{w3}^6}\right]^{1/6}, \quad g = r+C_{w2}\left(r^6-r\right), \quad r \equiv \frac{\tilde{\nu}}{\tilde{S}k^2d^2} \tag{18}$$

The closure coefficients for SA model [13] are $C_{b1} = 0.1355$, $C_{b2} = 0.622$, $\sigma_{\tilde{v}} = \frac{2}{3}$, $C_{v1} = 7.1$, $C_{w1} = \frac{C_{b1}}{k^2} + \frac{(1 + C_{b2})}{\sigma_{\tilde{v}}}$, $C_{w2} = 0.3$, $C_{w3} = 2.0$, $k = 0.4187$.

III. Result and Discussion

Prediction from the CFD simulation was compared to the Laser Doppler Anemometer (LDA) measurement by Bayly et al. [7] at various positions of the spray drying chamber. Data from CFD simulation were taken as a statistical average from up to 1000 time step after the pseudo convergence was achieved, which mimic the data collection in experimental measurement. Generally, all CFD models tested in this work can predict the flow pattern in counter-current spray drying reasonably well (Fig. 3). However, ultimate agreement was not achieved. The Rankine vortex due to the swirling flow was reproduced correctly.

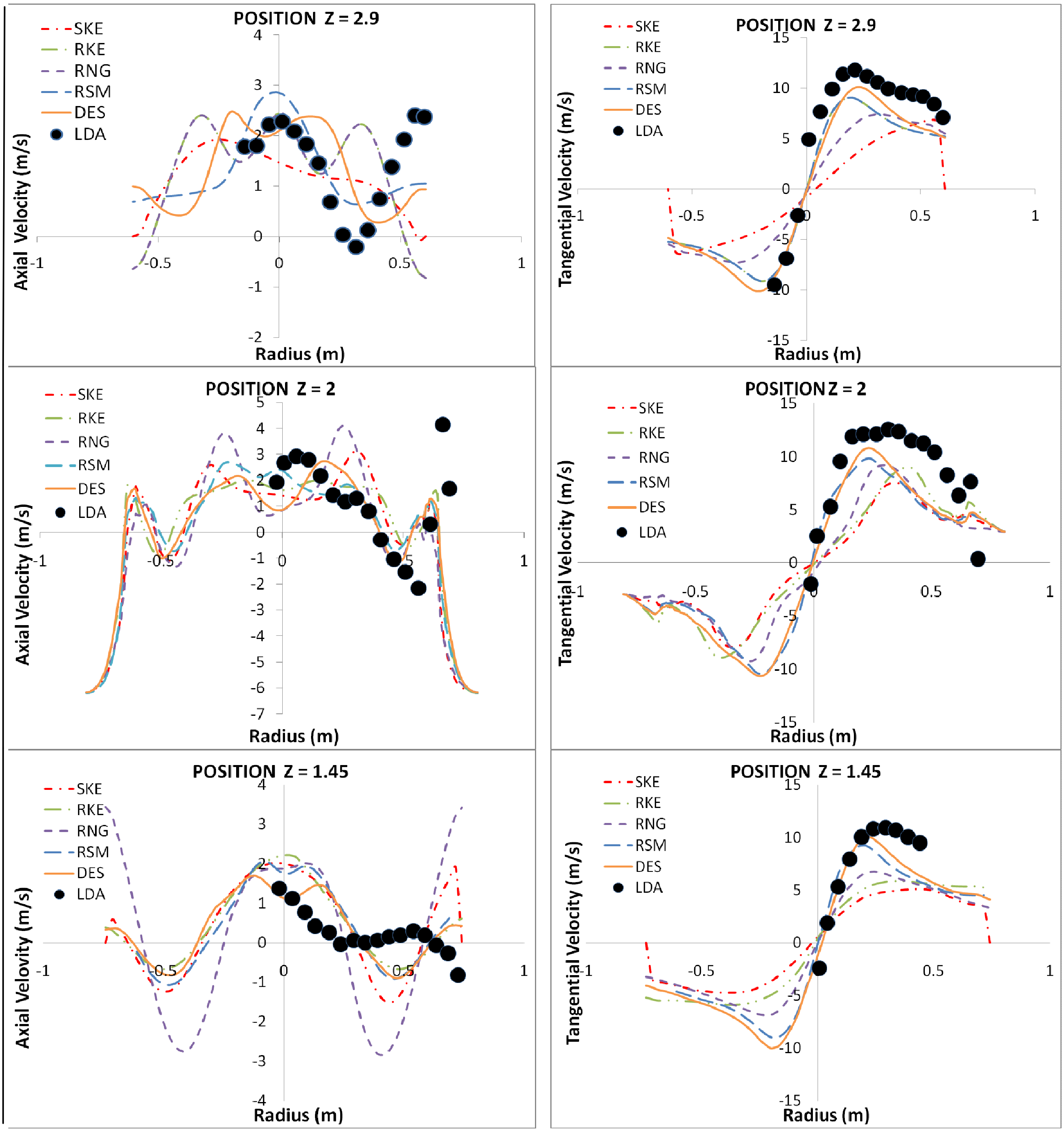

Figure 3: Prediction of axial and tangential velocity inside the counter-current spray dryer chamber using various turbulence models. Data points adopted from Bayly et al. [7]

Prediction by the DES model is by far the best among the model tested. This is attributed by the fact that DES employs LES in the bulk flow which in turn provides much better predictions of the turbulence flow. Around the boundary layer (i.e. the wall) the DES turn to a single equation Spalart-Allmaras turbulence model which provides a fair approximation of the flow near the wall without necessarily having to resolve the small eddies. This method of hybrid LES-RANS model employed in DES reduces the overall computational demand of a full LES solution while at the same time maintaining the prediction accuracy.

The RSM model outperformed all the other RANS based turbulence models (SKE, RKE and RNG) tested in this work. This is attributed by the anisotropic eddy viscosity model in RSM model, which is known for its excellent prediction for swirling and strong anisotropic turbulence flow such as in cyclone [14-15]. As it is mentioned in the previous section, the flow pattern inside the counter-current spray dryer studied in this work exhibit some swirling flow due to the position and design of the inlet gas around the tower hip, hence requiring a more complicated turbulence model for accurate prediction of the mean flow field inside the chamber.

The RNG model also predicts the tangential velocity fairly well, marginally better than the other two equations turbulence model of SKE and RKE. This is due to the inclusion of the swirl term in RNG model, which was not included in the SKE and RKE models. However, predictions obtained from these two-equation turbulence models which assume isotropic eddy viscosity were generally poor in comparison to either DES or RSM.

The axial flow pattern exhibit a single peak pattern similar to those normally seen for a reverse flow cyclone (e.g. Fraser et al., [16]). Again all models predict the axial flow pattern reasonably well compared to the experimental measurement. The DES and RSM models again provide much closer agreement to the experimental data in similar to the trend seen for the prediction of tangential velocity. Predictions by both RKE and RNG on the axial velocity are acceptable as the predicted value was relatively close to the experimental measurement. However, both RNG and RKE models may not be the best model for predicting the mean flow insider the counter-current spray dryer because they can produce somewhat unrealistic (triple peak) predictions on occasion as seen at Fig. 2 at Z =2.9 m. The SKE model was the worst among all the turbulence models tested, and hence should be avoided for modelling of a counter-current spray dryer.

IV. Conclusion

CFD simulation of a counter current spray dryer has been developed and predictions obtained using various turbulence models has uncovered a great potential of DES for modelling the flow field of the counter current spray dryer. Unfortunately, result from this simulation cannot be validated further due to limited data available for counter current spray dryer studied in this work. Results from this simulation may be useful for development of a more comprehensive and accurate model for counter current spray dryer in the future.

Acknowledgment

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APPENDIX B

CFD Simulation of Hydrodynamics in Counter-Current Spray Dryer Tower

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Abstract

Spray dryer is a well established method for converting liquid feed materials into dry powder forms. Spray dryer is widely used to produce foods such as whey, instant drinks, milk, tea and soups, as well as healthcare and pharmaceutical products, such as vitamins, enzymes, bacteria and also in production of fertilizers, detergent soap, and dyestuffs. Many experimental studies have been done to ensure the quality of the spray drying process. Alternatively, computational fluid dynamics (CFD) can be utilized to study the performance of the spray dryer. CFD modeling tools are increasingly used in the design, scale-up, optimization and trouble-shooting of the spray drying chamber because measurements such as Laser Droppler Anemometer (LDA) of air flow, temperature, particle size and humidity within the drying chamber are very difficult and expensive in a large scale spray dryer. Hydrodynamics of the counter-current spray dryer is not well understood and hence for economic and safety reasons, reliable models are needed for scale-up and design of such a spray dryer. In this work, a CFD modeling of hydrodynamics in a counter-current spray drying tower were performed. The turbulence modeling was realised using five different turbulent models, i.e. standard k-ε, RNG k-ε, Realizable k-ε, Reynolds stress models and the Detached Eddy Simulation. The predicted airflow patterns inside the spray drying chamber were found to be in good agreement to the experimental data adopted from literature for all turbulence models tested in this work. A great potential of the Detached Eddy Simulation for predicting the flow pattern in a counter-current spray dryer was uncovered as its provides more accurate predictions compared to other models tested in this work. Results from this simulation may be useful for development of a more comprehensive and accurate model for counter current spray dryer in the future.

Key words: Spray dryer, CFD, standard k-ε, RNG k-ε, Realizable k-ε, Reynolds stress models, Detached Eddy Simulation, Air flow pattern

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