

Computational Fluid Dynamics Modeling and Analysis of Lime Slurry Drying in a Laboratory Spray Dry Scrubber

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Cite This: *Ind. Eng. Chem. Res.* 2024, 63, 21038–21061



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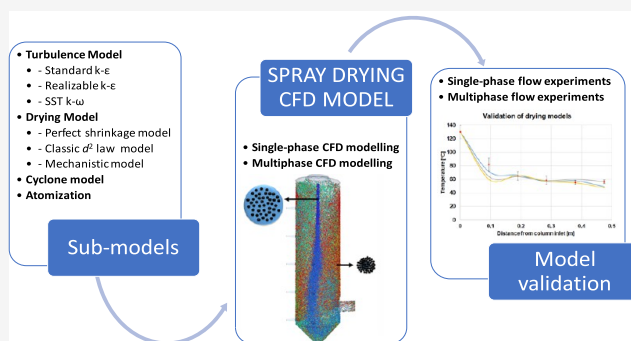


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ABSTRACT: Drying is an important process found in different industries including spray dry scrubbing as used in flue gas desulphurization. Understanding the fundamental processes in drying requires accurate description of turbulence and drying models, which is important in the design and optimization of new processes. Available research in spray dry scrubbing generally picks a single model to describe drying with the key assumption that it is relevant to the case being studied. This work does not make such an assumption but investigated the applicability of three drying models and three turbulence models in analyzing the drying process in a laboratory spray dry scrubber. Computational fluid dynamics was used to model the process employing the Euler–Lagrangian framework. The results from validated models showed that the investigated hindered drying mechanistic model is superior to the often used d^2 law and perfect shrinkage models and should therefore be used preferentially in drying applications.



1. INTRODUCTION

Flue gas desulphurization in spray dry scrubbing involves the exchange of heat and mass between a spray of alkali-based droplets and hot flue gas contacted cocurrently in a chamber. Different alkali-based sorbents are used—typical ones include calcium hydroxide (lime slurry), precalcined calcium oxide (limestone) and sodium carbonate; lime slurry is the most commonly used sorbent because of its cost effectiveness coupled with high reactivity toward sulfur dioxide.¹ In the process, sulfur dioxide is removed from the flue gas into the alkali-based droplets, wherein it reacts to form a sulphite salt. Simultaneously, water is removed from the droplets such that the product exits the chamber as dry particles, averting the need for downstream wastewater treatment and postprocess handling of a slurry product. The absorption of sulfur dioxide in a spray dry scrubber is dependent on the amount of water present in the droplets. The desulphurization efficiency of the flue gas is therefore limited by droplet drying dynamics.

In spray dryers, the atomized droplet/particle trajectory is influenced by the flow pattern of the continuous gas phase. The interaction also results in heat and mass transfer of water from the droplets and, consequentially, a cooling of the flow gas and change in its physical properties, and thereby its flow pattern. This indicates the coupled nature of the flow dynamics, which must be accurately captured in order to define this flow phenomenon.

Pioneering work on hydrodynamic modeling in spray dry scrubbing has often made simplifications of the flow pattern by assuming a completely back-mixed or two-dimensional (2D) plug flow pattern. The major challenge as highlighted by Mezhericher et al.² is that such a modeling approach fails to capture the intrinsic asymmetric nature of flow in spray drying systems and the impact of transversal flow on the drying dynamics. With an increase in computational capabilities, increasingly more modeling work has inclined toward computational fluid dynamics (CFD) modeling to better model the hydrodynamics and concurrently capture other complex phenomena, such as droplet atomization and representative turbulence occurring within the system. Jubaer et al.³ also refer to the capability of CFD in overcoming the limitations associated with analytical solutions. A review of CFD modeling in spray dry scrubbers has been reported by us earlier⁴ and a summary is presented in Section 2.

The choice of the applicable turbulence models needs to be made as part of the hydrodynamic modeling of spray dry scrubbers. Available models include the Reynolds-Averaged

Received: May 29, 2024

Revised: October 30, 2024

Accepted: November 13, 2024

Published: November 21, 2024



Navier–Stokes (RANS) based models, and in particular, the two parameter $k-\varepsilon$ and $k-\omega$ models, which are further described in Section 2.2. Poozesh et al.⁵ modeled the spray drying of active pharmaceutical ingredients using CFD. They investigated the use of the realizable $k-\varepsilon$ and shear stress transport (SST) $k-\omega$ turbulence models in the simulation of the process and concluded that the realizable model better captures swirl at the nozzle and results in more stable residuals of the conservation equations. However, they did not validate this with experimental data. In their work, a rigorous amendment of the characteristic drying rate curve method is proposed and implemented in modeling the droplet drying kinetics. A detailed description of the atomization details is also provided. However, only the particle size distribution was compared for model validation. Weiler et al.⁶ determined the evaporation time of water droplets in a modified BUCHI B290 spray dryer and compared results from a variety of simpler modeling approaches to CFD modeling results. They only used the realizable $k-\varepsilon$ model to describe turbulence in their work and only considered the drying kinetics of pure water droplets. In addition, the CFD results were only validated using a single variable, which was the exit gas outlet temperature. Despite ongoing research work on turbulence modeling, there is still no single model that is applicable to all flow situations—the appropriate model for any application is determined by judgment.

In terms of droplet drying dynamics, two drying approaches are generally followed in modeling the water removal from multiphase droplets in spray drying. Details of these models are presented in Section 2.3 and to the best of the authors' knowledge, the droplet drying mechanism has not received much attention in the CFD modeling of spray dry scrubbers. The comprehensive comparison of these models on the spray dryer performance has not yet been explored/reported in the available literature. In the present study, three models—the perfect shrinkage model, the classic d^2 law model and the mechanistic model proposed by Hill and Zank⁸—were investigated and comparisons made with experimental data in order to determine the most suitable model to employ for the drying of lime slurry droplets within the spray dryer.

Limited work is reported in open literature on CFD modeling and analysis of spray dry scrubbing. However, for general spray drying process, several works are available (generally focused on the food processing and pharmaceutical industries).^{4,9–11} Studies on spray drying analysis have been conducted on laboratory scale,⁹ pilot scale¹⁰ and industrial scale.¹¹ The smaller laboratory dryer is usually preferred because of the ease of investigation, and quantity and cost of consumables required.

The BUCHI B290 laboratory spray dryer has been successfully used by researchers in spray drying analysis for a wide range of industries. Zotarelli et al.¹² investigated the production of mango powder from a fruit pulp solution using the same spray dryer. Kemp et al.¹³ used the dryer in the production of fine lactose particles from an organic solvent of ethyl acetate. Liu et al.¹⁴ used the dryer in synthesizing sorbents for carbon dioxide removal from mixtures of calcium oxide and various supporting precursors. With regards to modeling work on the dryer, Kemp et al.¹⁵ used CFD to study the spray drying of aqueous solutions of egg albumin; however, they do not provide the intrinsic modeling details of the work to allow for complete understanding of the hydrodynamics involved.

Despite ongoing efforts directed at CFD modeling of the spray dry scrubbing process, there remains a gap in terms of sufficient hydrodynamic modeling of the process harnessing the

full power of CFD, in particular, the ability to analyze the multiphysics, multiphase and multiscale flow processes occurring inside the spray dry scrubber—then thereby offering a better understanding of the complex phenomena. When it comes to the topic of spray drying, for which significant CFD modeling has been done, the main challenge remaining in most of the published literature is the lack of rigorous model validation with experimental data.

This work therefore aims at addressing this shortcoming by presenting an analysis that validates the CFD model in a systematic manner within the modeling framework—commencing with single-phase model validation and then amending the validated model to a multiphase drying model, which is then also validated. Such a model will then form an initial framework for the incorporation of the complex desulphurization reaction mechanism as further work—thus lending more confidence to the model accuracy and its predictive capability. In this study, a modified laboratory-scale BUCHI B290 mini-spray dryer was used to study the spray drying of lime slurry using CFD as an analysis tool. Single-phase modeling of the continuous gas phase traversing the spray chamber, including the attached downstream cyclone as an additional submodel, was studied and an investigation of the appropriate turbulence model for this study was undertaken. Validation using experimental data measured radially and axially along the column, as well as at the column exit outlet leg, was conducted. The single-phase model was then amended to include the dispersed phase in the form of atomized slurry droplets and the Euler–Lagrangian framework was used to model the interaction of the different phases. The predictive capability of three models of droplet drying kinetics was investigated and the results compared with experimental data. An evaluation of the robustness of the developed CFD model in predicting the temperature within the column, the exit gas temperature, the exit particles' average moisture content, at different inlet gas temperatures and liquid to gas (L/G) flow rates, was also conducted.

The work carried out in this study therefore sought to address, first, the selection of the appropriate turbulence model for the employed laboratory spray dryer. It proceeded to investigate the applicable drying model—a deviation from the assumption made in previously published work in spray dry scrubbing, where a single model is used to describe the mechanism without prior analysis on the model's applicability on the investigated application. The work then concludes with analyzing the accuracy of the developed CFD model in predicting selected operational parameters.

2. LITERATURE REVIEW

2.1. CFD Modeling. CFD has widely been accepted as a modeling tool that is able to provide accurate prediction of the complex processes in multiphase fluid systems. Pertaining to the CFD modeling of the spray dry scrubbing process, Katolicky and Jicha¹⁶ used CFD to model flue gas desulphurization in a laboratory spray dry scrubber using a two-fluid nozzle with the size spectrum of the atomized droplets characterized using the Rosin-Rammler distribution. They used a commercial CFD platform (StarCD) in their work solving the conservation equations of heat, mass and momentum using the Eulerian framework for the continuous phase and the Lagrangian framework for the dispersed phase. They only considered the impact of drag and gravity on the Lagrangian phase and used the Schiller–Neumann correlation to model the drag coefficient. Only convective heat transfer and associated evaporative effect

between the phases was taken into consideration and the Ranz and Marshall correlation was used to define the heat transfer coefficient for the Lagrangian particles. The RANS model was used with a stochastic eddy interaction model to analyze the motion of the droplets and the standard $k-\epsilon$ closure models were employed. The details on the discretization and pressure–velocity scheme were not presented in the study. The work was validated using results of previous experiments reported by Hill and Zank.⁸ Later, Katolicky and Jicha¹⁷ modeled the desulphurization process in an industrial-scale spray dry scrubber using a rotary atomizer in a CFD platform. The size spectrum was assumed, the droplet Sauter mean diameter was inferred from a previous study and the initial tangential droplet velocity given by the rotational speed, while the radial component was calculated by an empirical correlation. The details of other intrinsic phenomena such as particle–wall interaction were not provided in the work; only the final sulfur dioxide removal efficiency as a means of validating their model is reported. More recently, Mei et al.¹⁸ modeled an industrial-scale spray dry scrubbing process using CFD modeling. They used the commercially available Ansys CFX (16.0) for CFD analysis and the Eulerian–Lagrangian framework to solve the mass and momentum conservation equations. Their work modeled a rotary atomizer and simplified the atomization process by looking at monosized particles entering the column at a tangential wheel velocity. The study considered the impact of drag and gravity in modeling the Lagrangian phase motion and used the Schiller–Neumann correlation to model the drag coefficient. The renormalized group-based (RNG) $k-\epsilon$ equations were used in the modeling of turbulence in the scrubber. A more rigorous wall impingement model was utilized, however, the drying model used ignores the impact of Stefan flow on the evaporation process: the latter is particularly critical in drying operations. The generated grid used in their study comprised of an unstructured tetrahedral mesh which was further refined where the injection pores were located. The first order upwind convection scheme and central difference diffusion scheme were used in the discretization of the turbulence formulations. In the present work these shortcomings are addressed in developing a comprehensive CFD model for a laboratory spray dry scrubber.

2.2. Turbulence Models. In spray drying, various turbulence models, mostly using the simplified RANS time-averaged-based method, have been employed by different authors. In its formulation, the RANS method includes a time-averaged component and a fluctuating component; the latter may be described by different models, usually referred to as closure models.¹⁹ The two-equation models ($k-\epsilon$ and $k-\omega$ models) are the most commonly used, with the most rigorous model, and therefore computationally more expensive, being the Reynolds stress model (RSM); it utilizes seven equations for its closure models.²⁰ The robustness of the standard $k-\epsilon$ model to simulate the spray drying process has been proven by many authors²¹ who have used the model in their work and reported good agreement with experimental data, such as Katolicky and Jicha¹⁶ and Kavoshi et al.²² The realizable $k-\epsilon$ model and renormalization group method model, adaptations of the standard $k-\epsilon$ model to better capture recirculation, swirl and flow separation within the dryer,²⁰ have also been used successfully in spray drying work.^{18,23,24} The $k-\omega$ models are known to better model near-wall effects, where the $k-\epsilon$ models have failed.²⁵ Longest et al.⁹ used the $k-\omega$ model in their work and validated the study with experimental data. More recently,

an adaptation of the $k-\omega$ models, the SST $k-\omega$ model, developed by Menter²⁵ and associates, has gained prominence in spray drying work, particularly for counter-current operations. The SST $k-\omega$ model blends the $k-\epsilon$ and $k-\omega$ models to activate the $k-\epsilon$ model in the free stream region and the $k-\omega$ model at the near-wall region. Jubaer et al.²⁶ adjusted the model and demonstrated its effective use in predicting their experimental data. The RSM models, which are the most rigorous of the RANS models, have also been implemented in the spray drying process.^{11,27} Huang et al.,²⁸ Langrish,⁷ and Jubaer et al.²⁶ provide comparative studies of the different turbulence models in adequately predicting flow patterns in their respective works.

In the present work, the following three models were analyzed to determine the most suitable model for the lime slurry spray drying process: the standard $k-\epsilon$ model, realizable $k-\omega$ model and SST $k-\omega$ model. Choice of the investigated turbulence models was informed by the computational expense while the selection process was guided by the quality-of-fit to experimental data, with the final selected model judged by the lowest root-mean-square error (RMSE) among other criteria.

2.3. Drying Models. An extensive review of the different drying models applicable in spray dry scrubbing was recently reported and compiled by the authors.⁴ The review showed that two approaches may be used in modeling the drying kinetics of droplets containing suspended or dissolved solids. The first approach is to treat the slurry droplets as pure water droplets and model the water removal as purely by evaporation, assuming that the dissolved or suspended solids within the droplet do not hinder the removal rate. The second approach considers the hindrance of the particles within the slurry droplet on the water removal rate.

The models generated from the former approach, hereafter referred to as evaporation models, in their simplest form may be represented as the perfect shrinkage model, where the impact of the moving flow and/or droplet on the evaporation rate and the effect of Stefan flow on the rate are disregarded. The variation of such a model is the classic quasi-steady state model, also known as the classic d^2 law, which incorporates Stefan's flow on the removal rate. The d^2 law may also be amended to include other complexities such as spatial gradients and transient conditions within the droplet. Sirignano²⁹ gives further details on these amendments.

The latter modeling approach takes into account the different drying regimes that are a consequence of the solid's hindrance on evaporation, and may be referred to as hindered drying modeling. The hindered drying models may be classified into lumped parameter models, internal diffusion-based models and mechanistic models. The lumped parameter models do not consider the liquid-phase resistance on the water migration rate, while internal diffusion-based models track the moisture gradient within the droplet. The mechanistic models may also track the water migration within the droplet but usually avoid the rigorous solution of the partial differential equations associated with the more accurate internal diffusion-based models.⁴ Despite this, the mechanistic models should have improved capability for describing the water removal process at lower computational cost. Although the second modeling approach best represents the droplet drying mechanism in spray dry scrubbers, the modeling complexities associated with their implementation make it computationally costly, particularly in a process that already comprises other complex phenomena such as chemical reactions. Most published CFD

Table 1. Conservation Equations Used in the Numerical Analysis for the Continuous and Dispersed Phases

continuous phase (Eulerian framework)	equation
mass	$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \cdot \bar{u}) = S_m \quad (1)$
species	$\frac{\partial (\rho \cdot w_A)}{\partial t} + \nabla \cdot (\rho \cdot w_A \cdot \bar{u}) = \nabla \cdot (\rho \cdot w_A \cdot D_{AB}) + S_{mA} \quad (2)$
momentum	$\frac{\partial (\rho \cdot E)}{\partial t} + \nabla \cdot (\rho \bar{u} E) = -P \nabla \cdot \bar{u} + \nabla \cdot (k_c \cdot \nabla T) + \rho \bar{u} \bar{g} + S_E \quad (3)$
energy	$\frac{\partial (\rho \cdot \bar{u})}{\partial t} + \nabla \cdot (\rho \bar{u} \times \bar{u}) = -\nabla P + \nabla \cdot (\tau - \tau^R) + \rho \cdot \bar{g} + S_{\text{mom}} \quad (4)$
dispersed phase (Lagrangian framework)	equation
trajectory	$\frac{d\bar{x}}{dt} = \bar{v} \quad (5)$
mass	$\frac{dm_d}{dt} = S_{k,m} \quad (6)$
momentum	$m_d \cdot \frac{d\bar{v}}{dt} = S_{k,\text{mom}} + m_d \cdot \bar{g} \quad (7)$
energy	$m_d \cdot C_{p,d} \cdot \frac{dT_d}{dt} = S_{k,E} \quad (8)$

modeling work on spray dry scrubbing processes has resorted to the first modeling approach.

Mei et al.¹⁸ used the perfect shrinkage model to account for the water removal rate from the droplets injected into an industrial-scale spray dry scrubber using a rotary atomizer. Katolicky and Jicha¹⁶ later use the classic d^2 law to model the drying rate from slurry droplets in an industrial scale spray dry scrubber. Hill and Zank⁸ use a hindered drying mechanistic model to describe the water removal rate, which Katolicky and Jicha¹⁶ incorporate in their CFD work to describe the drying process of the slurry droplets in a laboratory-scale spray dry scrubber. However, the effectiveness of the model in predicting the water removal rate is not indicated. The present work proceeds by evaluating and comparing these three drying models.

3. NUMERICAL MODELS

The Euler–Lagrange framework was used to model the interaction of gas and droplets, wherein the gas was modeled as the continuous phase and described using the Eulerian approach, while the spray of slurry droplets was modeled as the dispersed phase and thus described using the Lagrangian approach.

3.1. Governing Equations. The governing equations of mass, heat and momentum conservation (eqs 1–4) for the continuous phase are given in Table 1. in the Eulerian framework, where S is any additional source (or sink) term of mass, species, energy or momentum. In order to calculate the source terms for the continuous phase, all contributions of individual Lagrangian particles within a cell volume were volume averaged.

The dispersed phase eqs (eqs 5–8) are also given in Table 1. The indicated source terms in the equations were deduced from the models given in the subsequent sections, where the mass transfer of water from the droplet to the gas phase was modeled using three different drying models.

3.2. Turbulence Models. The standard k – ε models use two variables, the turbulent kinetic energy (k) and the turbulence dissipation coefficient (ε) for closure equations, and are given in eqs 9–10:

$$\begin{aligned} & \frac{\partial (\rho \cdot k)}{\partial t} + \nabla \cdot (\rho \cdot k \cdot \bar{u}) \\ &= \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \cdot \nabla k \right] G_k + G_{nl} + G_b - Y_M - \rho \cdot \varepsilon + S_k \end{aligned} \quad (9)$$

and

$$\begin{aligned} & \frac{\partial (\rho \cdot \varepsilon)}{\partial t} + \nabla \cdot (\rho \cdot \varepsilon \cdot \bar{u}) \\ &= \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \cdot \nabla \varepsilon \right] + C_{1\varepsilon} \cdot \frac{\varepsilon}{k} \cdot (G_k + G_{nl} + C_{3\varepsilon} G_b) \\ & - f_2 \cdot C_{2\varepsilon} \cdot \rho \cdot \frac{\varepsilon^2}{k} + S_\varepsilon \end{aligned} \quad (10)$$

where G_k is the generation term of the turbulent kinetic energy due to the averaged velocity gradients and G_b due to the buoyancy, with G_{nl} being the nonlinear contribution of the generation term. σ_k and σ_ε are the turbulent Prandtl numbers and S_k and S_ε are the source terms. Y_M is the contribution of compressible component of turbulence and f_c the curvature correction factor. $C_{1\varepsilon}$, $C_{2\varepsilon}$, and $C_{3\varepsilon}$ are model associated constants.

The Realizable k – ε models also use the k and ε as closure equations, and they may be given by eqs 11–13:

$$\begin{aligned} & \frac{\partial (\rho \cdot k)}{\partial t} + \nabla \cdot (\rho \cdot k \cdot \bar{u}) \\ &= \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \cdot \nabla k \right] + f_c \cdot G_k + G_b - Y_M - \rho \cdot \varepsilon + S_k \end{aligned} \quad (11)$$

and

$$\begin{aligned} & \frac{\partial(\rho \cdot \varepsilon)}{\partial t} + \nabla \cdot (\rho \cdot \varepsilon \cdot \vec{u}) \\ &= \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \cdot \nabla \varepsilon \right] + C_{1\varepsilon} \cdot \frac{\varepsilon}{k} \cdot (f_c \cdot S_k + C_{3\varepsilon} \cdot G_b) \\ & \quad - f_2 \cdot C_{2\varepsilon} \cdot \rho \cdot \frac{\varepsilon^2}{k} + S_\varepsilon \end{aligned} \quad (12)$$

The μ_t is the turbulent or eddy viscosity, calculated as follows:

$$\mu_t = \rho \cdot C_\mu \cdot f_\mu \cdot \frac{k^2}{\varepsilon} \quad (13)$$

where C_μ is an empirical constant and f_2 and f_μ are damping functions that enforce realizability.

The SST k - ω model, use k and the specific dissipation rate (ω) given by eqs 14–18:

$$\begin{aligned} & \frac{\partial(\rho \cdot k)}{\partial t} + \nabla \cdot (\rho \cdot k \cdot \vec{u}) \\ &= \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \cdot \nabla k \right] + P_k - \rho \cdot \beta^* \cdot \omega \cdot k \end{aligned} \quad (14)$$

$$\begin{aligned} & \frac{\partial(\rho \cdot \omega)}{\partial t} + \nabla \cdot (\rho \cdot \omega \cdot \vec{u}) \\ &= \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\omega} \right) \cdot \nabla \omega \right] + \alpha \cdot P_\omega - \rho \cdot \beta \cdot \omega^2 \\ & \quad + 2\rho \cdot (1 - F_B) \cdot \frac{1}{\sigma_{\omega,2}\omega} \cdot \nabla k \cdot \nabla \omega \end{aligned} \quad (15)$$

where μ_t is given as

$$\mu_t = \rho \cdot \frac{k}{\omega} \cdot \min \left(\alpha^*, \frac{a_1 \cdot \omega}{\zeta \cdot F_E} \right) \quad (16)$$

And the generation of the turbulent kinetic energy (P_k) and the dissipation rate (P_ω) described as

$$P_k = \min(\mu_t \cdot \zeta^2, 10\rho \cdot \beta^* \cdot k \cdot \omega) \quad (17)$$

$$P_\omega = \frac{P_k}{\min \left(\frac{k}{\omega}, \left(\alpha^*, \frac{a_1 \cdot \omega}{\zeta \cdot F_E} \right) \right)} \quad (18)$$

F_E and F_B are blending wall functions and ζ is the invariant strain rate. β^* and β are turbulence model constants and α^* and a_1 are flow transition constants.

3.3. Mass Transfer–Droplet Drying Models. Three droplet drying models were investigated in this study. The first of the models, the perfect shrinkage model, is defined from eq 19, as follows:

$$\frac{dm}{dt} = -Sh \cdot \pi \cdot \rho \cdot D_{H_2O,g} \cdot d_d \cdot (w_{H_2O,\infty} - w_{H_2O,s}) \quad (19)$$

The second model is the classic d^2 law model, given by eqs 20–22, as follows:

$$\frac{dm_d}{dt} = -Sh \cdot \pi \cdot \rho \cdot D_{H_2O,g} \cdot d_d \cdot \ln(1 + B_M) \quad (20)$$

where B_M is the Spalding transfer number given as

$$B_M = \frac{w_{H_2O,\infty} - w_{H_2O,s}}{1 - w_{H_2O,\infty}} \quad (21)$$

and the Ranz and Marshall correlation used to compute the mass transfer coefficient is as follows

$$Sh = \frac{k_{H_2O,g} \cdot d}{D_{H_2O,g}} = 2 + 0.6 \cdot Re_p^{0.5} \cdot Sc^{0.33} \quad (22)$$

The third drying model, the mechanistic model, is formulated from eqs 23–27, as follows:

$$\frac{dm_{H_2O}}{dt} = \rho_g \cdot A_d \cdot K_{H_2O,c} \cdot \ln \left[\frac{1 - y_{H_2O,\infty}}{1 - y_{H_2O,s}} \right] \quad (23)$$

where

$$\frac{1}{K_{H_2O,c}} = \frac{1}{k_{H_2O,c}} + \psi \quad (24)$$

and

$$\psi = \frac{1}{\left(\frac{S_{d_i,d_{ag}} \cdot D_{H_2O,g}}{\epsilon \cdot A_{ag}} \right)} \text{ if } x \leq x_c \quad (25)$$

$$\psi = 0 \text{ if } x > x_c \quad (26)$$

where x_c defines critical conditions identified in this work with a filling coefficient of 74% solids volume fraction within the droplet.¹⁶ At this point, the water interphase is assumed to recede into the droplet and the solids hindrance on the water removal rate becomes pronounced. The tortuosity parameter is given as ϵ , and the geometric parameter $S_{d_i,d_{ag}}$ is defined as

$$S_{d_i,d_{ag}} = \frac{2\pi}{\frac{1}{d_i} - \frac{1}{d_{ag}}} \quad (27)$$

3.4. Momentum Transfer. The momentum balance was computed using eq 28, as follows:

$$\frac{d\vec{v}}{dt} = C_D \cdot \frac{18 \cdot \mu}{\rho_p \cdot d} \cdot \frac{Re_p}{24} \cdot (\vec{u} - \vec{v}) + g \cdot \left(\frac{\rho_p - \rho}{\rho_p} \right) + \sum F_i \quad (28)$$

where F_i in this work accounts for the pressure gradient force (F_{PG}), shear lift force (F_L), and added mass force (F_{AM}) given in eqs 29–31.

$$F_{AM} = \frac{\rho \cdot V_p}{2} \cdot \left(\frac{D\vec{u}}{Dt} - \frac{d\vec{v}}{dt} \right) \quad (29)$$

$$F_{PG} = -V_p \cdot \nabla P_{static} \quad (30)$$

$$F_{SL} = C_{SL} \cdot \frac{3V_p}{4} (\vec{\omega} \times \vec{u}) \quad (31)$$

where $\vec{\omega}$ is the curl of the fluid velocity and the coefficient for the lift force (C_{SL}) is given by the Sommerfeld correlation³⁰ which is robust for a broad range of Reynolds numbers. The drag coefficient is defined by the Schiller–Neumann correlation (eqs 32 and 33), which is applicable for small-diameter solids and liquid droplets³¹ and used successfully in previous work on spray drying and spray dry scrubbing^{16,18,24} for cocurrent operation.

$$C_D = \frac{24(1 + 0.15 \cdot Re_p^{0.687})}{Re_p} \dots \text{for } Re_p \leq 1000 \quad (32)$$

$$Re_p \equiv \frac{\rho \cdot |\bar{u} - \bar{v}| \cdot d_{\text{droplet}}}{\mu} \quad (33)$$

3.5. Heat Transfer. The energy balance was computed using eqs 34 and 35, as follows:

$$m_d \cdot C_{p,d} \cdot \frac{dT_d}{dt} = Nu \cdot \lambda \cdot \pi \cdot d \cdot (T - T_d) + h_{\text{vap}} \cdot \dot{m}_d \quad (34)$$

with the Ranz and Marshall correlation used to compute the transfer coefficient

$$Nu = \frac{h \cdot d}{\lambda} = 2 + 0.6 \cdot Re_p^{0.5} \cdot Pr^{0.33} \quad (35)$$

4. MATERIALS, EXPERIMENTAL METHODS, AND COMPUTATIONAL APPROACH

4.1. Material and Experimental Methods. A laboratory BUCHI B290 mini-spray dryer having a spray chamber diameter of 0.48 m and a height of 0.154 m, was modified in order to enable the axial and radial measurements required for the study. The modifications included installation of five sampling pots each separated by a distance of 0.095 m along the column length and at two positions, 90° apart, around the column. Figures 1

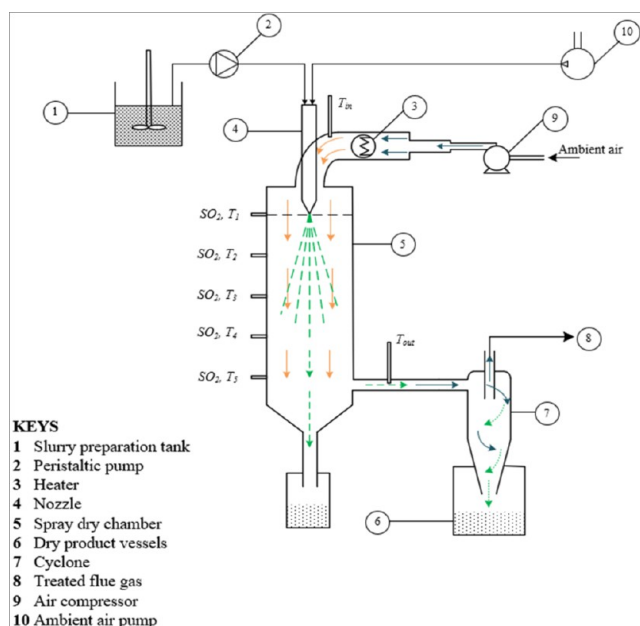


Figure 1. A schematic diagram of the spray drying of slurry in the BUCHI B290 laboratory spray dryer used in this work, with green lines showing cold streams and orange lines showing hot streams (adapted in part with permission from B-290 Spray Dryer operation manual.³² Copyright 2018 BÜCHI Labortechnik AG).

and 2 show a schematic of the dryer setup showing the sampling pot levels and locations. Detailed equipment and operational specifications of the dryer are available in the BUCHI B290 mini-Spray Dryer Operation Manual.³² Single-phase flow experiments followed by multiphase flow experiments were conducted (see Sections 4.1.1 and 4.1.2 for details) at inlet temperature conditions suitable for flue gas desulfurization

which have also been used by previous researchers⁸ and L/G flow rates as limited by the equipment design parameters. The sprayed lime slurry sorbent used for the multiphase flow experiments was also characterized, as reported in Section 4.1.3.

4.1.1. Single-Phase Flow Experimentation. The single-phase experiments were conducted in order to validate the implemented model hydrodynamics and, particularly, to inform the choice of turbulence model for the current spray system. Air was introduced into the heating chamber using an air compressor able to supply a maximum of 35 m³/h volumetric flow rate, before it entered the spray chamber. The compressed air was heated to operating temperature using an electric heater with a rated capacity of 2.3 kW and temperature control achieved using a PT100 fuzzy logic controller having a manufacturer stated accuracy of ±2 °C. The inlet temperature of the air was recorded at six locations around the inlet annulus and the average temperature was noted. The air traversed the column and heat was lost to the environment. The temperatures of the air across (radial temperature measurements) and along (axial temperature measurements) the spray chamber were recorded at five positions along the column length (Figure 2), once the column outlet temperature reading and a single temperature reading within the column had stabilized. The air then exited the column, where the exit temperature was measured before the air entered the cyclone. It then traversed the cyclone and exited at ambient pressure conditions.

4.1.2. Multiphase Flow Experimentation. Figure 1 shows the multiphase flow interaction of the heated air with the sprayed slurry droplets within the BUCHI B290 spray dryer chamber. The spray dryer was fitted with a two-fluid nozzle (nozzle tip 0.7 mm, cap size 1.5 mm). A lime slurry of known concentration was prepared and atomized into a chamber, where it was contacted cocurrently with heated air. Hydrated lime and distilled water were used to prepare the slurry samples of known concentrations. Details of characterization of the hydrated lime (sorbent) are presented in Table 2. Upon contact with the heated air, the moisture content of the slurry droplets is reduced and the final particles are separated from the cooled air stream in a cyclone. Axial and radial temperature measurements of the air stream were recorded at five positions along the column length and at the cyclone exit (T_{out}) for model validation. In the experiments conducted, the temperature was measured using an external thermocouple together with the in-built BUCHI B290 spray dryer thermocouples. After obtaining steady temperature values, the runs were all performed in triplicate and a mean temperature value recorded. Air temperature measurements within the column were facilitated by utilizing an amended microseparator device, as designed by Kievit,³³ for the multiphase flow case.

Part of the experimental work included determining the particle size distribution (PSD) of the produced spray dryer solid product. This was achieved through the laser diffraction technique using the Malvern Mastersizer 2000.

4.1.3. Sorbent Characterization. Commercial grade hydrated lime sorbent supplied by Kayla Africa Suppliers and Distributors CC (South Africa) was used in this study. The hydrated lime had a density of 2210 kg/m³ and was mixed with distilled water to make a 10 wt % solids slurry used for the experimental work. It was further characterized by X-ray fluorescence (XRF) analysis and X-ray diffraction (XRD) analysis; results are tabulated in Table 2 and also show the loss on ignition (LOI). XRF analysis was carried out using an XRF spectrometer (Model MiniPAL 4 Brand: PANalytical PW4030). XRD analysis was performed using a Malvern

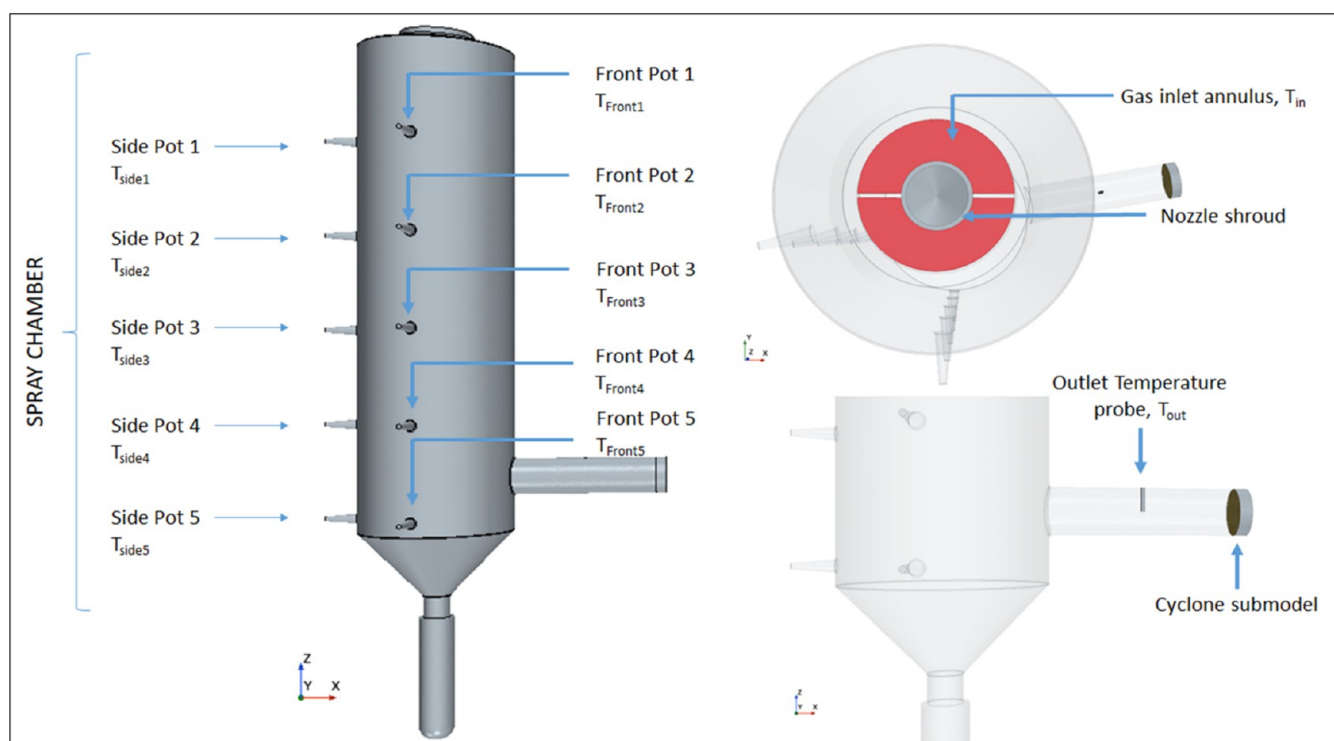


Figure 2. Geometric representation of the modified laboratory spray dryer showing the new side and front pots, enabling radial and axial measurements as implemented in STAR-CCM+.

Table 2. XRF and XRD Analyses of Hydrated Lime Used in this Work (Adapted from Ref 34)

XRF content (wt %)					
CaO	SiO ₂	MgO	Al ₂ O ₃	Na ₂ O	LOI
58.5	4.8	0.7	0.5	0.2	35.0
XRD content (wt %)					
portlandite (Ca(OH) ₂)		calcite (CaCO ₃)		quartz (SiO ₂)	
86.9		12.2		0.9	

Panalytical AERIS diffractometer with a PIXcel detector having slits fixed with Fe-filtered Co- $K\alpha$ radiation. The resultant phases were determined using X'Pert High score software.

XRF analysis (Table 2) gave calcium to be the major component of the hydrated lime sample and XRD analysis gave portlandite (Ca(OH)₂) to be the major component. Further numeric modeling undertaken in this study therefore considered the slurry solids to be Ca(OH)₂.

4.2. Computational Approach. Implementation of the numerical models described in Section 3 was undertaken using STAR-CCM+ (v.16.02.008) CFD software. The modeling approach used in this work followed a two-step process. First the CFD hydrodynamic model, incorporating the different turbulence models as discussed in Section 3.2, was set up and the turbulence model best describing column hydrodynamics was chosen through validation of the model with experimental data. The selected model was subsequently employed in the second step, which involved the introduction of the dispersed phase into the domain and where the three different drying models (described in Section 3.3) were compared and validated with experimental data. Such a modeling approach as followed in this work has the advantage that it allows for systematic validation of the applicable models, thereby increasing the confidence of the developed CFD model in adequately describing the spray drying

process. This is achieved by confirming the hydrodynamics prior to the model complexity introduced by the incorporation of the dispersed phase in the simulation. The complexity of the modeling approach employed in this work was further increased by the inclusion of the cyclone at the outlet of the scrubber, which inherently affects the pressure drop and thus the hydrodynamics within the chamber.

For both the single-phase and multiphase modeling, as per steps one and step two described above, an unsteady state modeling framework was preferred to the steady state approach as the solution method. This was informed by previous work which showed that the usual approach of initiating such solutions by first running a steady state framework until partial convergence and then using the resultant solution as an initial estimate of the transient model output did not always give realistic results and, at times, led to nonconvergence.³ As such, the solution commenced by running a transient simulation for the single-phase model until a fully developed flow and convergence was achieved, as judged by the residuals which had to be reduced to below 1×10^{-4} , as well as achieving a relatively constant gas temperature leaving the scrubber. Thereafter, the time was rezeroed upon the addition of the dispersed phase, as the multiphase simulations were initiated. Subsequently, the model was run to convergence, which was judged as per the single-phase case, as well as achieving a relatively constant particle count inside the dryer and a relatively constant outlet moisture content of the exit gas. The overall mass and energy balance also had to be satisfied as part of the convergence criteria.

The segregated flow solver was used to resolve the pressure–velocity coupling with a first order upwind convection scheme. The AMG linear solver with Gauss–Seidel relaxation scheme was employed to solve the segregated flow, species and energy equations.

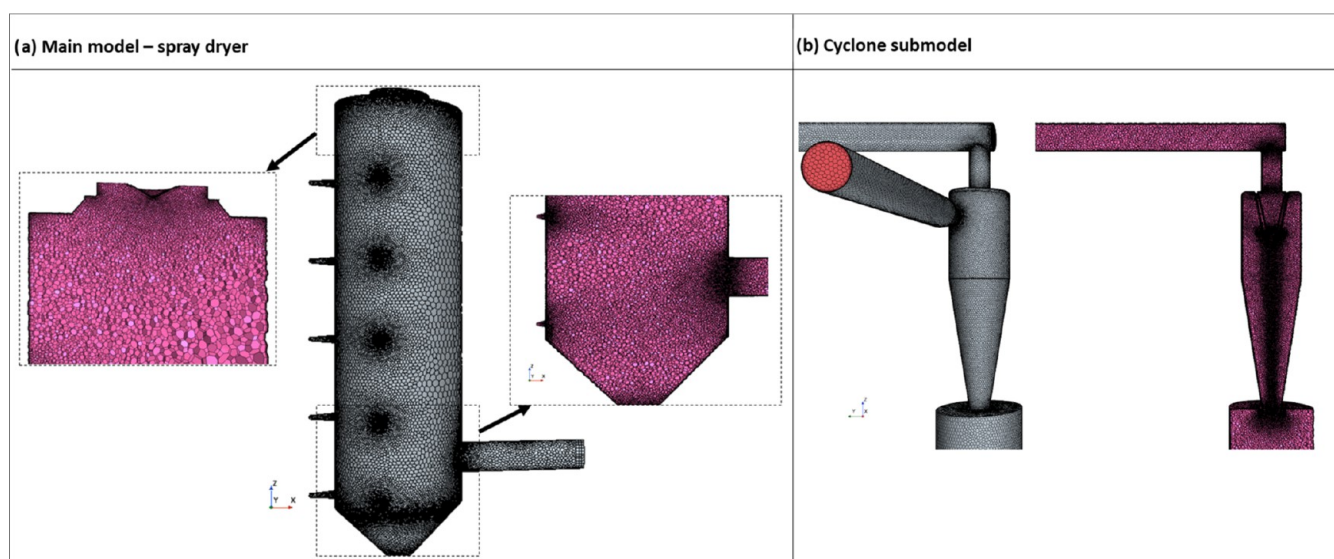


Figure 3. Controlled volumetric mesh representation of (a) the main model and (b) the cyclone submodel, generated in STAR-CCM+.

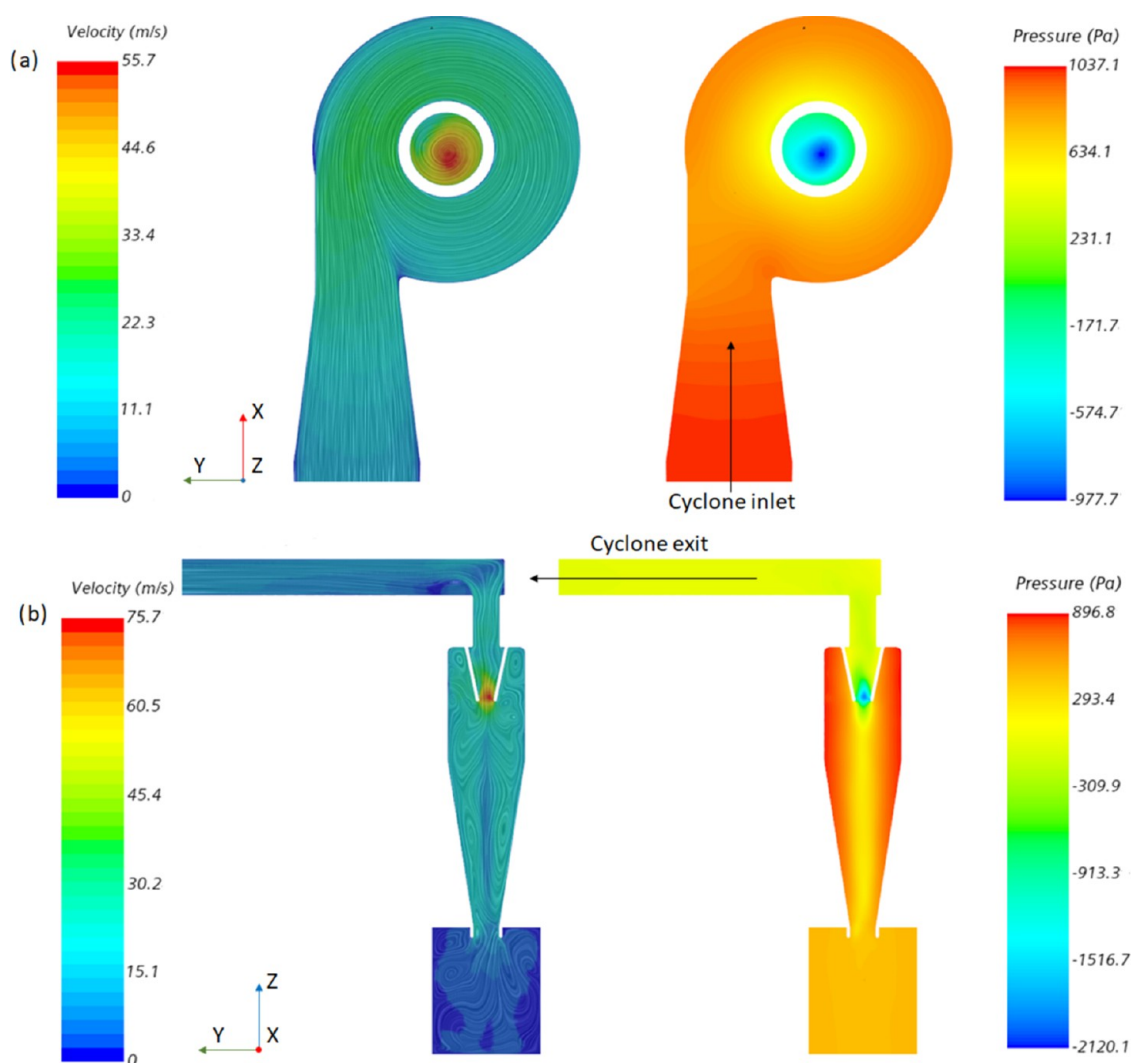


Figure 4. Cyclone submodel velocity and gauge pressure profiles: (a) along the x – y plane, (b) along the y – z plane, as incorporated into the main spray dryer model to capture the cyclone influence on the chamber dynamics.

4.2.1. Single-Phase Flow Modeling Approach. A polyhedral mesh (see Figure 3), with eight prism layers and surface

remesher, was used to generate a volumetrically controlled mesh with 2468780 cells. An ideal and compressible gas was modeled.

The turbulent flow of the gas was investigated using three models: the standard $k-\epsilon$ model, the realizable $k-\epsilon$ model and the SST $k-\omega$ model. The segregated fluid temperature was used to capture energy transfer. Heat loss through the column wall was also modeled, with a defined borosilicate glass thermal diffusivity of 0.74 W/mK³⁵ and a heat transfer coefficient of 5 W/m²K—a value given by Welty³⁶ for natural convection and confirmed by Hanus and Langrish³⁵ for its applicability to the BUCHI B290 spray dryer within the temperature ranges investigated in this study.

A submodel of the cyclone was also included and its influence on the chamber hydrodynamics captured in the form of an extrusion located at the spray column outlet leg (see Figure 2). The RSM turbulence model was used for the cyclone submodel in order to correctly capture the prevalent highly anisotropic flow behavior seen in cyclones.^{37,38} Typical results, depicted in Figure 4, were obtained from the cyclone model; results, showed a uniform tangential velocity through the cyclone inlet, which increased in the radial direction toward the column center and then sharply through the vortex finder. The chaotic nature of the flow was perceived from the axial velocity profile, where high swirling was observed. The gauge pressure profiles exhibited a drop toward the column center, displaying a vortex core, which is characteristic in cyclone design.³⁹ The velocity and pressure profiles were then used in determining the resistance function of the extrusion; the loss coefficient was calculated assuming the pressure drop was purely inertial and implemented in the form of a resistance which varied as a function of the superficial velocity when characterizing the extrusion properties.

The initial and boundary conditions of the investigated simulation study are summarized in Table 3, where the inlet

Table 3. Initial and Boundary Conditions Used for Single-Phase Modeling and Amendment to Include the Dispersed Phase for Multiphase Modeling

parameter	units	value
continuous phase		
inlet boundary—velocity inlet		hot gas
inlet temperature (based on experimental measurements)	°C	108.8; 130.3; 142.5
inlet L/G ratio	-	0.04; 0.05; 0.03
outlet boundary—pressure outlet		exit gas
dispersed phase		
inlet boundary—velocity inlet		atomization air
relative humidity (at 20 °C)	%	24
mass flow rate	kg/h	0.5
dispersed phase—Injection properties		(10 wt % solids) lime slurry
mass flow rate	kg/s	1.1
temperature	°C	20

boundary (implemented as a velocity boundary) the outlet boundary (implemented as a pressure boundary) and wall conditions are detailed; submodel details are also given.

4.2.2. Multiphase Flow Model Modeling Approach. The converged single-phase model was successively adapted to include an injection of droplets into the domain. The Euler–Lagrangian framework was used to model the continuous gas phase and the dispersed slurry droplet phase, respectively. The two-film nozzle atomizer was implemented into the model as a full cone spray with a 44° angle, as determined from the work of Poozesh et al.⁴⁰ A Rosin–Rammmler particle size distribution with a mean droplet size of 10.5 μm and spread parameter of 4.9

was determined using the back calculation method⁴¹ and 80 parcels were used to represent the spray field. The atomization gas was included in the model by creating a species mass source on a select volume of cells surrounding the nozzle. The Schiller–Neumann model was used to account for the drag force; virtual mass and shear lift forces were also included. The droplets were allowed to rebound at the walls with a normal and tangential restitution coefficient. Stuck droplet heat and mass transfer were also modeled via the Rohsenow correlation. The perfect shrinkage model, the classic d^2 law and the mechanistic model were investigated for their prediction of the temperature and water removal rate from the slurry droplets within the domain. Table 3 gives a summary of the multiphase flow boundary conditions as implemented in the model.

Following the identification of the applicable droplet drying model among the three investigated models, one-at-a-time factor investigations were undertaken, where the inlet temperature was varied while keeping the L/G ratio constant, and subsequently keeping the temperature constant while varying the L/G ratio. This is further discussed in Sections 5.2.2–5.2.4. Table 6 shows the details of the different case studies.

4.2.3. Grid and Time Independence Analysis. A conventional grid independence test was done for this work, where the predicted temperature inside the column was compared to the measured values at key points along the column, and the observed variation used to determine the chosen mesh size. The grid independence test was conducted for three mesh sizes made up of a course-sized grid having 537,429 cells, a medium-sized grid having 2,468,780 cells and a fine grid having 3,178,420 cells corresponding to 0.02, 0.01, and 0.005 mm cell base sizes, respectively. The predicted CFD model temperature results (sampled axially along the column length at 4 cm from the wall) were then used to determine the optimum grid and results are shown in Figure 5.

From the results in Figure 5a,b there is no significant change in the predicted temperatures for both the single-phase and multiphase models moving from the medium grid to the fine grid and therefore the medium-grid resolution was chosen for this study taking into account the increased computational expense from working with the fine grid. In addition, the optimum grid resolution was judged through comparing the RMSE (defined in eq 36) obtained by comparing the measured values to the model-predicted results for the investigated temperatures. The values obtained for the single-phase and multiphase cases of the RMSE are shown in Figure 5c. These also indicate that there is no significant change in decreasing the cell size from the medium to the fine grid.

In terms of the time independence analysis, the Courant number was used to judge the model independence to the selected time step. Figure 5d shows the volume fraction of the cells as a function of the convective Courant number and indicates that more than 96% of the cells in the simulation volume had Courant numbers less than one, and 99.9% less than 3, thus generally satisfying the acceptance criteria of a Courant number less than one.

5. RESULTS AND DISCUSSION

5.1. Single-Phase Flow Model Results. 5.1.1. Air Flow Field. The resultant air flow field within the dryer for the single-phase flow model is given in Figure 6, which depicts the air streamlines upon entry into the spray chamber. Distinctive attributes such as the air flow deflection, recirculation, and vortex formation are noted and highlighted.

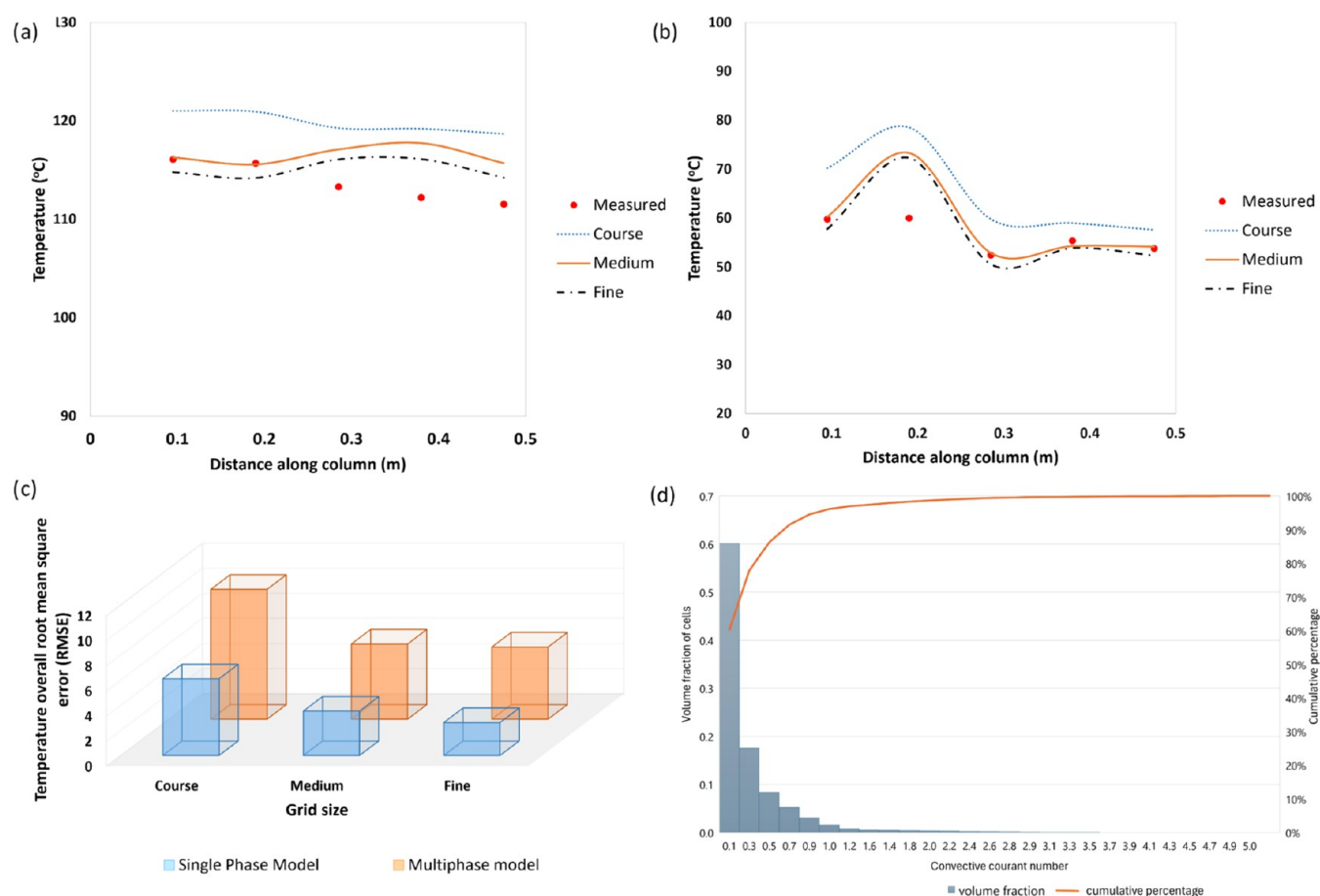


Figure 5. Grid and time independence analysis for the CFD Model developed in this study.

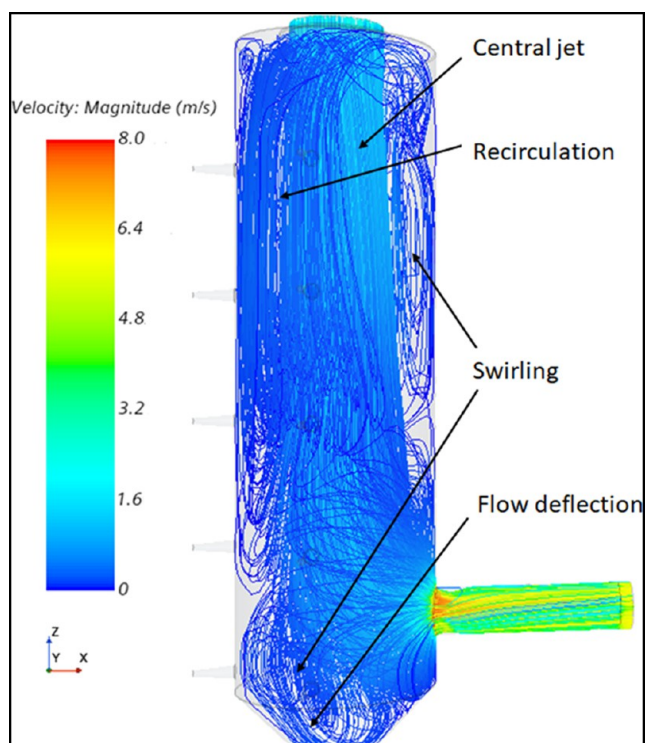


Figure 6. Single-phase flow field streamlines realized after 10 s simulation flow time, indicating the velocity magnitude and showing the flow deflection, swirling and recirculation within the dryer.

An intact central jet core is seen to be sustained from the chamber inlet through to the outlet leg (Figure 6), where some of the flow finds its way to the exit leg. The conical section of the chamber acts as a deflection plate, diverting some of the air reaching the bottom of the chamber out through the leg. A portion of the air is directed upward along the column wall where it recirculates before exiting the column; some vortex formations are also seen because of this recirculation. Similar flow patterns have been observed in other studies^{3,5} with different dryer configurations. According to earlier reported works, the particles/droplets predominantly follow the gas pathways,¹⁰ making it important to predict with much accuracy the applicable turbulence model for the study. This is discussed in more detail in Section 5.1.2.

5.1.2. Turbulence Model Validation. This section provides a comparison of the turbulence models investigated as discussed in Section 4.2. The models were compared with each other and to the experimental data; results are shown in Figures 7 and 8, respectively.

Three RANS-based turbulence models were investigated (see Section 3.2). Figure 7 shows a comparison of the velocity profiles for the three turbulence models that were investigated. Looking closely at Figure 7a, showing the velocity on the y - z plane, some differences are evident in the observed flow patterns of the different turbulence models. The inlet central jet for the standard k - ϵ model is seen to dissipate early along the length of the column, followed by the realizable k - ϵ , with SST k - ω displaying the longest dissipation time. In terms of the observed higher velocity dissipation (associated with a shorter dissipation

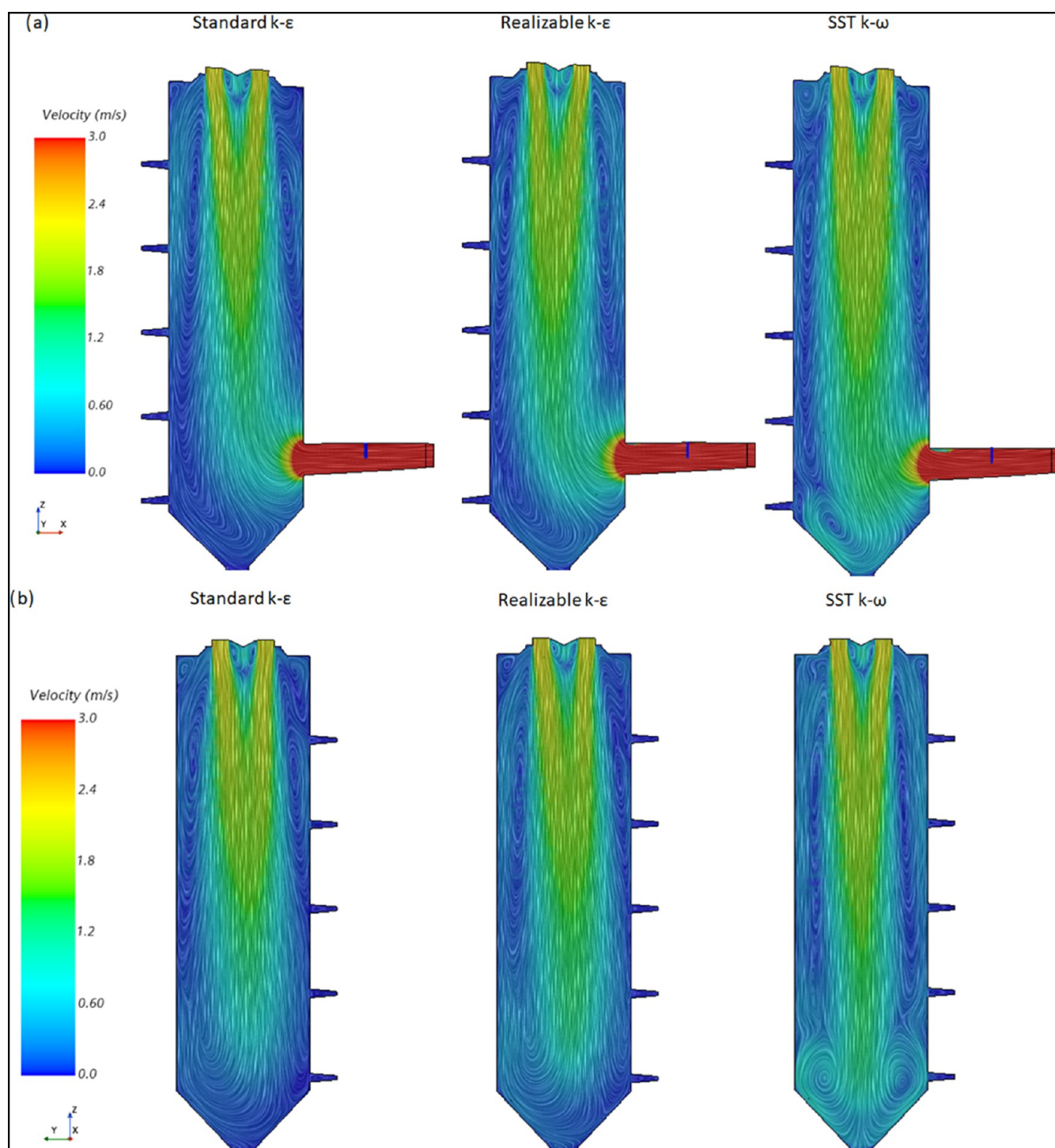


Figure 7. Comparison of the velocity contour plots on the x - z (a) and y - z (b) planes generated by the different turbulence models for the single-phase flow modeling after 10 s simulation flow time.

time) for the $k-\epsilon$ models, this is likely due to the over prediction of the wall effects by these models when compared to the SST $k-\omega$ model. The observed high impact on the velocity is thus due to the over prediction of the wall shear stress. These models therefore result in increased velocity attenuation given that they are not derived to adequately capture the boundary layer effects as was also previously shown by²⁵. Increased radial and axial mixing with the standard $k-\epsilon$ model compared with the other models is observed. Another notable feature observed in Figure 7a is that the SST $k-\omega$ model, followed by the standard $k-\epsilon$

model, captures increased recirculation at the top of the column. At the bottom of the column the SST $k-\omega$ model shows distinct recirculation post the deflection of the central jet after impinging the conical section of the column—a phenomenon partially evident in the flow patterns of the other turbulence models. All the models show a similar flow pattern—a central jet down the column and recirculation toward the column wall and at the bottom of the column. The x - z plane, as shown in Figure 7b, also shows similar patterns, with the standard $k-\epsilon$ model closely resembling the realizable $k-\epsilon$ at the bottom section of the tower.

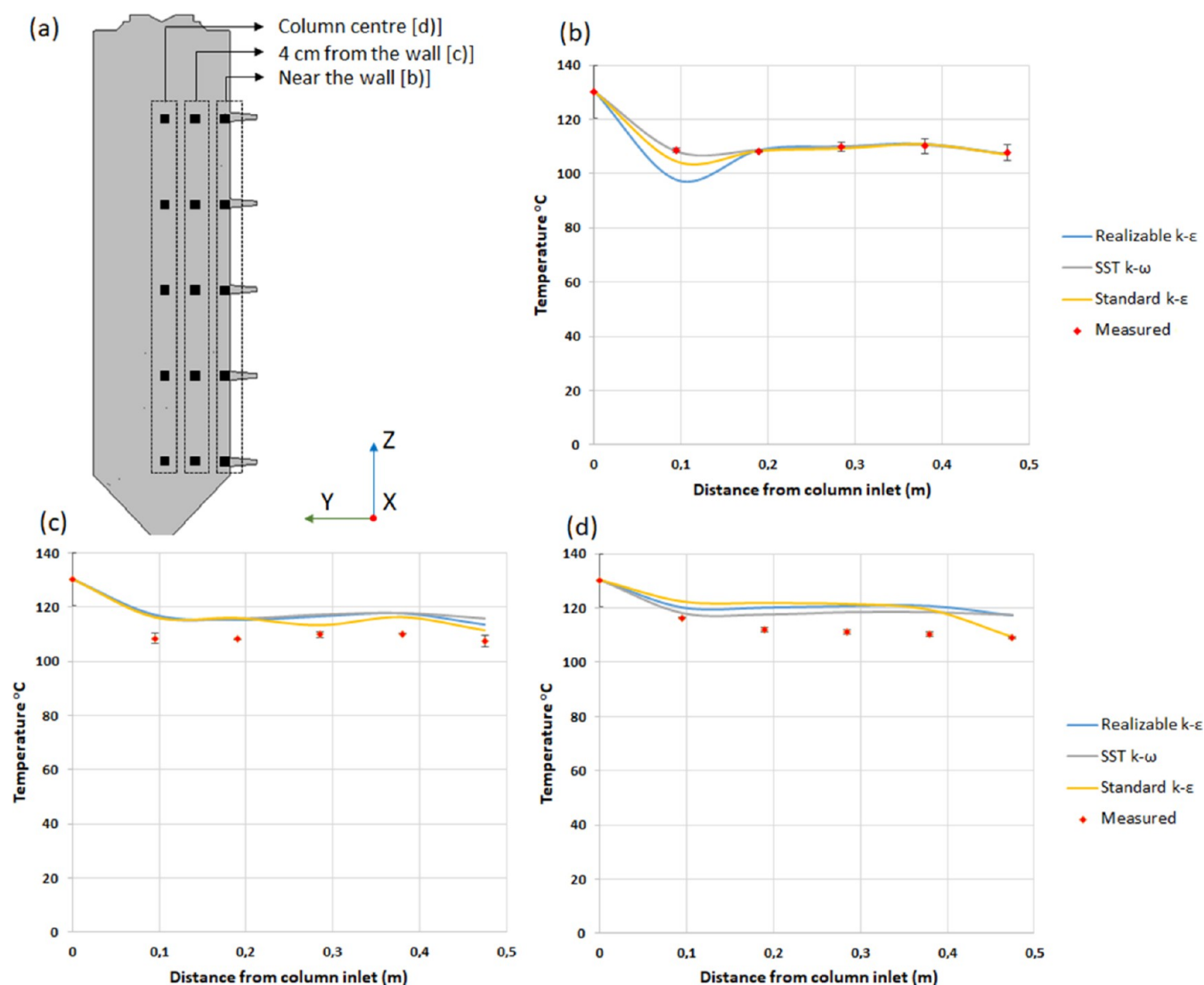


Figure 8. (a) Column y - z plane showing temperature measurement locations and temperature prediction plots of the different turbulence models along the column (where zero is the top of the column): (b) near the column wall, (c) 4 cm from the wall, and (d) at the column center. Comparison with experimental data is included.

For the bottom section of the column in this plane, the SST k - ω model shows intricate swirling that is not seen in the k - ϵ models. This is because the SST k - ω model in its derivation and also as has been shown in its applicability, is better suited to describe such separating flows and hence results in better capture of the swirling motion in that section of the chamber. The results obtained in terms of the turbulence model representation of the flow characteristics inside the column are in line with published literature reporting the greater capability of the standard k - ϵ models in predicting the free stream velocity and the SST k - ω model in predicting near-wall effects, flow separation and recirculation as a consequence of adverse pressure gradients^{4,26} resulting from the deflection of flow by the conical section of the column.

The foregoing discussion indicates that the flow dynamics as predicted by the SST k - ω model, although similar to the k - ϵ models, noting (as already highlighted) that it blends the k - ϵ and k - ω models to activate the k - ϵ model in the free stream region and the k - ω model near the wall region, manages to better capture the expected swirling and recirculation in the column. The final selection of the best turbulence model was

done through validation using measured temperature, as presented in Figure 8.

Next, the indirect method of validating the flow field with temperature was employed—similar to in the work of Jubaer et al.²⁶ Figure 8 shows the temperature profiles of the three turbulence models at three radial positions within the chamber and along the column, compared with experimental values. Notably, near the column wall and at 4 cm from the wall (Figure 8a,b), there is an initial decrease in the air temperature upon entry into the chamber, followed by an increase in the middle section of the chamber and then a decrease toward the chamber exit. The increase is attributed to the mixing of the cold and hot air due to the recirculation patterns that were noted in this section of the column, where mixing of the inherently hot central jet with the recirculating lower temperature air takes place (Figure 7). A different trend is seen at the center of the column, where there is a gradual reduction in the temperature of the air from the chamber inlet to the outlet (Figure 8c), typical to an intact central jet core with limited mixing, as it traverses down the column. The noted decrease can be explained by the nonadiabatic nature of the process. All the turbulence models

Table 4. Quality-of-Fit of the Three Turbulence Models Compared with Experimental Data for Single-Phase Flow Analysis

single-phase flow		flow within the chamber				flow exiting the chamber		
investigated turbulence models	quality-of-fit of temperature [°C]	distance from the wall			overall RMSE	model T_{out} [°C]	measured T_{out} [°C]	% error – model T_{out}
		near the wall	4 cm from wall	column center				
standard $k-\epsilon$	RMSE	1.8	2.0	6.9	4.3	111.5	108.9	2.4
realizable $k-\epsilon$	RMSE	4.5	3.2	7.1	5.2	101.2	108.9	7.1
SST $k-\omega$	RMSE	0.4	3.0	5.8	3.8	108.2	108.9	0.6

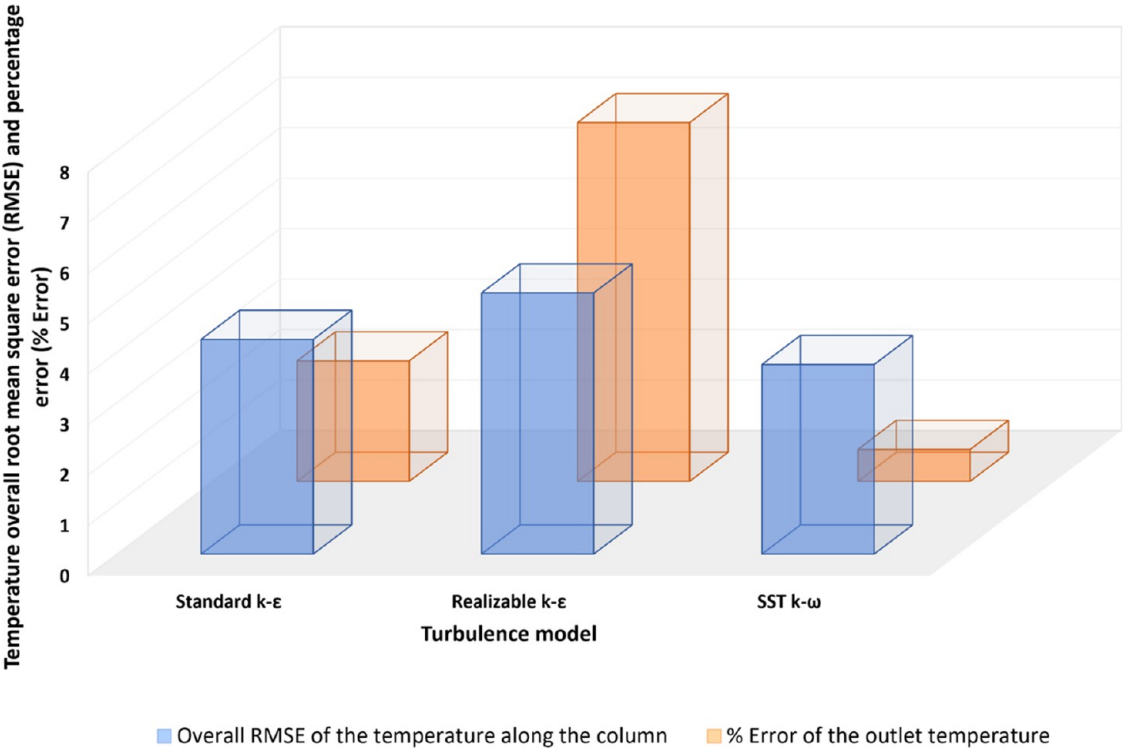


Figure 9. Comparison of the different turbulence models used for single-phase analysis.

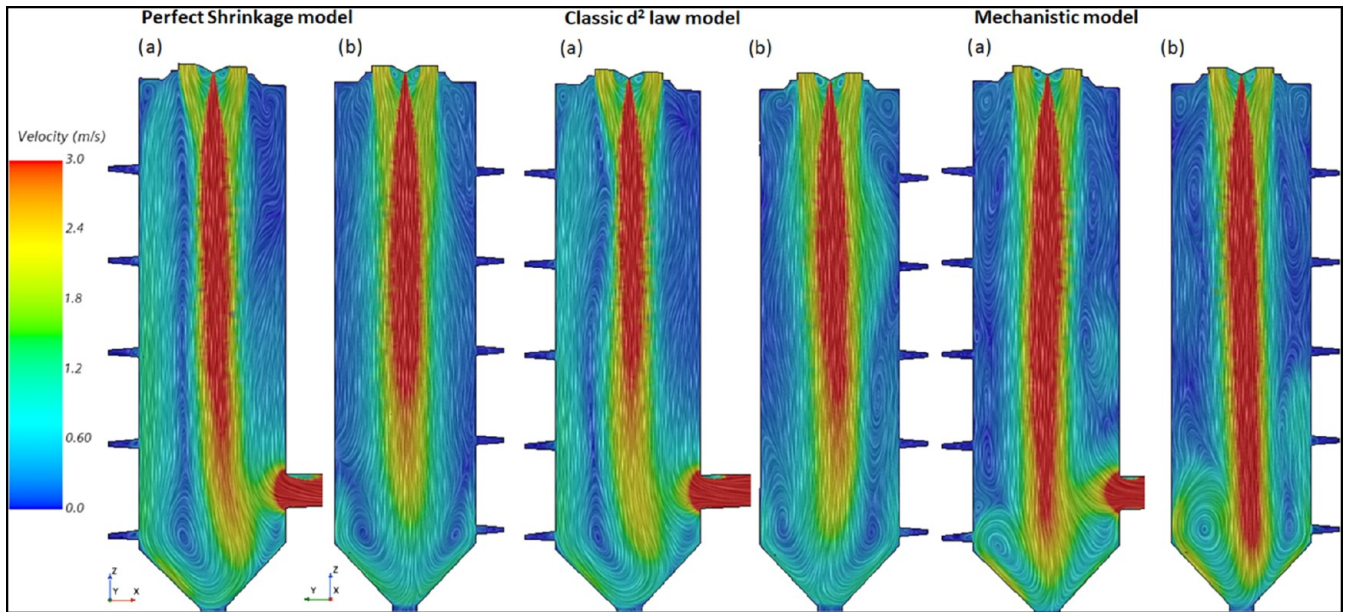


Figure 10. Comparison of the resultant velocity contour plots on the (a) x - z plane and (b) y - z plane for the different drying models of the multiphase flow modeling after 10 s of Lagrangian injection flow time.

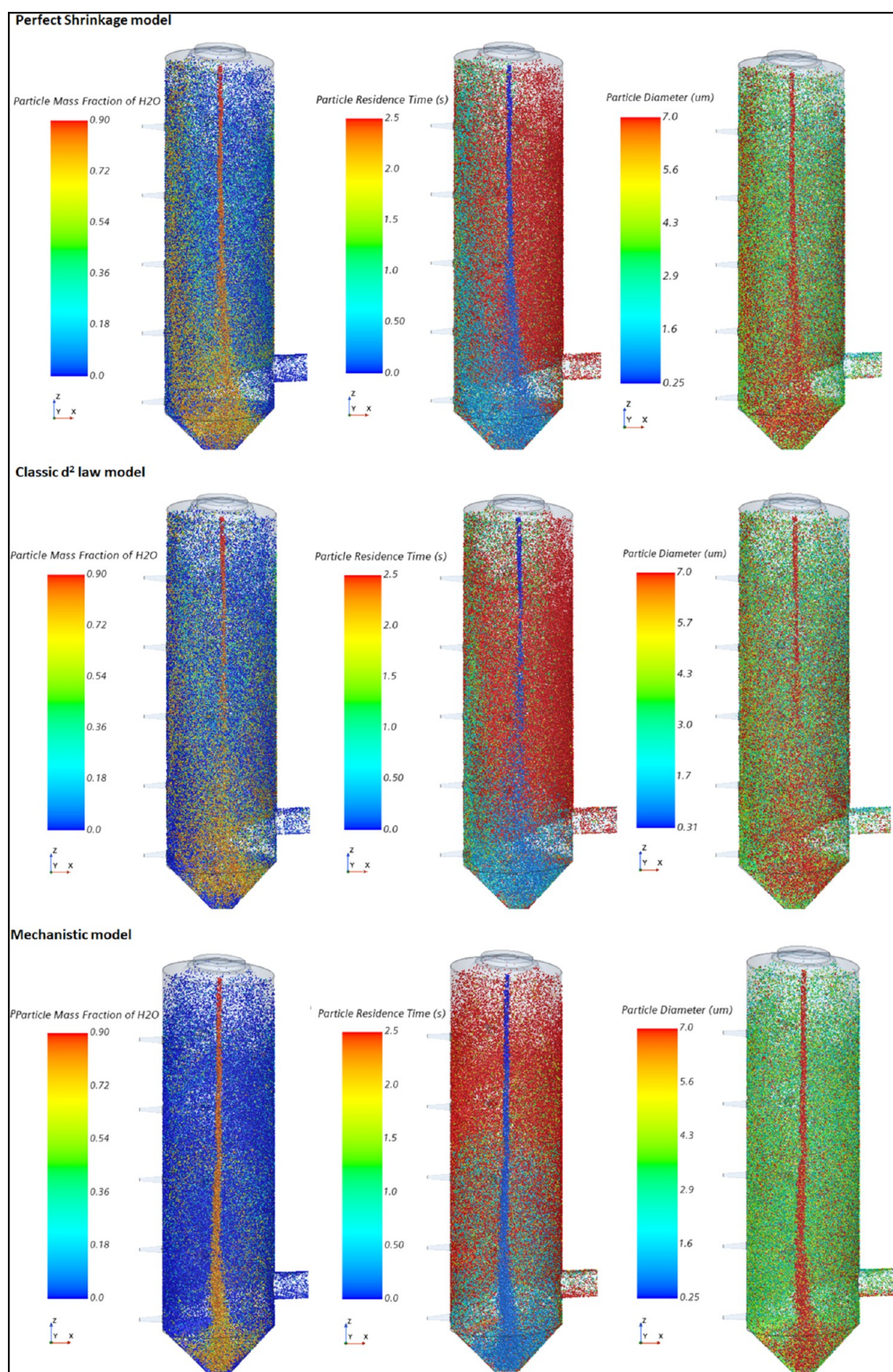


Figure 11. Central section snapshot along the x - z plane for the different drying models showing the droplet mass fraction, particle residence time and diameter of the droplets/particles for the multiphase flow modeling after 10 s of Lagrangian injection flow time.

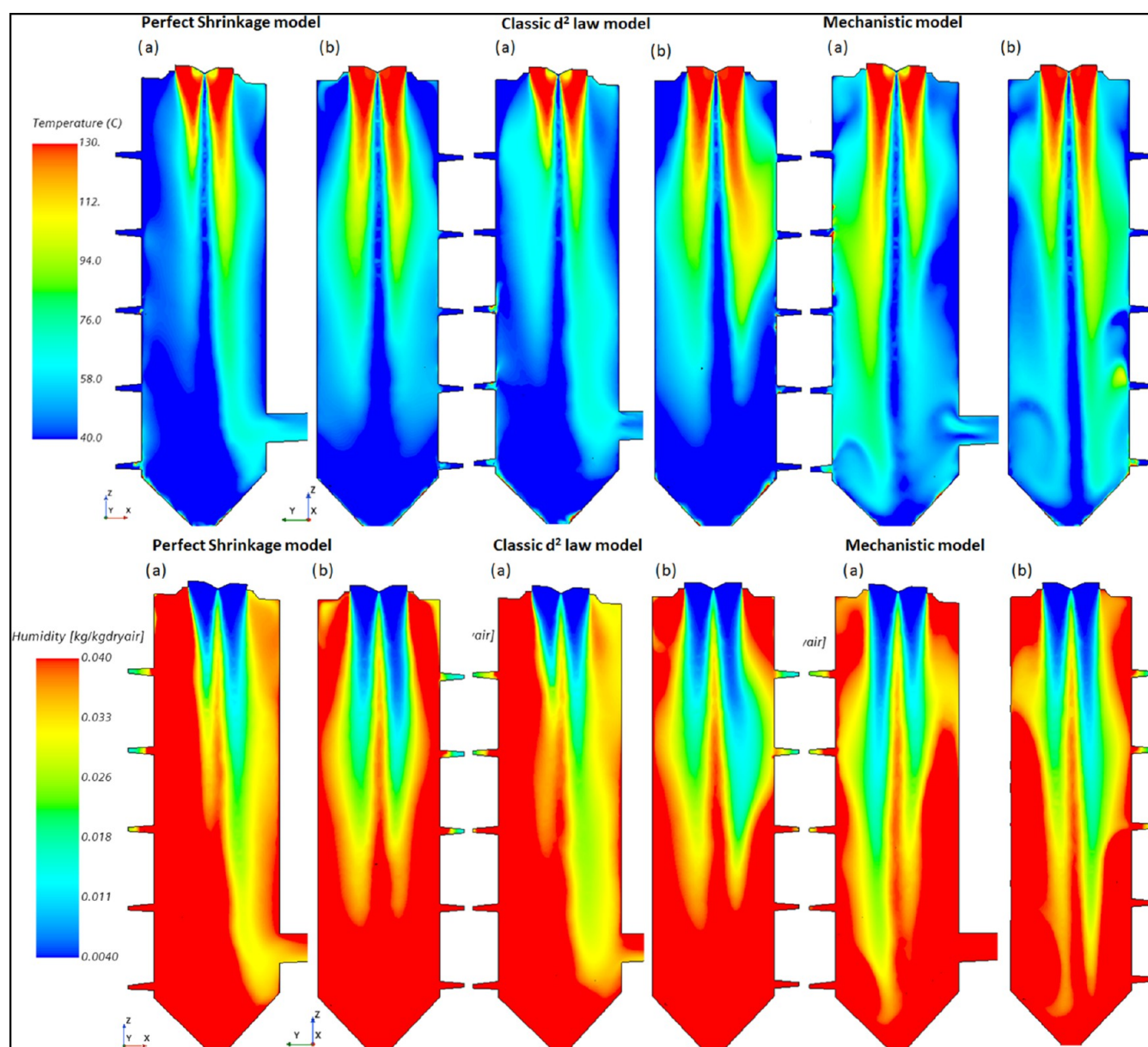


Figure 12. Comparison of the resultant temperature and humidity profiles generated by the different drying models of the multiphase flow modeling after 10 s of Lagrangian injection flow time: (a) along the x - z plane, (b) along the y - z plane.

predict a similar trend-capturing the effect of the recirculation on the flow field for the near-wall region and a sluggish decrease toward the column center.

Two metrics (eqs 36 and 37) were used to assess the quality-of-fit of the three turbulence models to the experimental data: the RMSE and the percentage error of the average temperature:⁴²

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (36)$$

$$\% \text{Error} = 100 \times \frac{|\hat{y}_i - y_i|}{\hat{y}_i} \quad (37)$$

where n is the number of observations, y_i the observed values and $\hat{y}_i$ the model-predicted values.

The metrics were then used to identify the turbulence model, which would be used further in the study for the subsequent

multiphase modeling. The results are shown in Table 4 and a visual representation in Figure 9. The models seem to better predict the conditions near the wall than at the center of the column, as evident from the relatively high RMSE values at the center of the chamber compared with those at the wall. Earlier work has reported discrepancies of central simulation results with experimental data;²⁶ this is attributed to inadequate mixing of the central jet with the recirculating air. The same discrepancies, particularly on the predicted and observed outlet temperatures, have recently been reported by Milanesi et al.,⁴³ who compared two different modeling approaches for the same spray dryer as used in this work; the highest reported RMSE was 7.21. The same deduction indicating better prediction with the SST k - ω model may be made when noting the lower percentage error of the outlet temperature when compared with that of the other models. Based on the magnitude of the overall RMSE, the order of the models in terms of representation of the experimental data is then as follows: the SST k - ω model, the

standard $k-\varepsilon$ model and, last, the realizable $k-\varepsilon$ model. The SST $k-\omega$ model was thus selected for the remainder of this work.

5.2. Multiphase Flow Model Results. The multiphase flow modeling approach was discussed in Section 4.2.2, wherein the dispersed phase injection into the domain was implemented subsequent to running the single-phase model to convergence. For the selected turbulence model, the resultant velocity profiles are shown in Figure 10. Figure 11 shows a snapshot of the droplets/particles inside the dryer, detailing the mass fraction, residence time and droplet diameter of the particles. Further details of the drying process and analysis of moisture content are discussed in Section 5.2.1. In this Section 5.2, the flow and temperature profiles that were obtained from the model are presented, together with other modeling results.

Closer examination of Figure 10 shows that all drying models show an intact central jet stream from the chamber inlet down the conical section of the column, similar to the behavior observed in the single-phase flow cases (Figure 7). The high velocity of the central jet compared with to the rest of the gas in the column is a result of the high atomization air velocities used in the nozzle. Although the width and length of the central jet vary for the different models, pronounced changes are seen in the results for the perfect shrinkage and the classic d^2 law drying models, where there is a slight deflection of the jet at the bottom of the column as it is rerouted toward the outlet of the chamber. Furthermore, as expected, the flow velocity of the air is seen to increase through the exit leg to the cyclone due to the sudden contraction in the cross-sectional area for all models. The central jet dissipates at the bottom of the column where it impacts the conical section with a portion of it deflecting back toward the top, where it recirculates, creating vortices in its path. This is clear in both the perfect shrinkage and the d^2 law models, although there is evidence of bias toward the outlet ports ($-x$ axis) in the $x-z$ plane compared with in the mechanistic model. The flow field as predicted by the mechanistic model shows lower velocity gas flow close to the wall of the column compared with in the other two drying models. This is a result of the pronounced swirling in the mechanistic model at the conical section of the column, where the bulk of the velocity of the gas is dissipated and hence lower velocity recirculation streamlines are seen rising toward the top of the column.

The slurry used in this work was fed into the chamber at a 10 wt % solids concentration. The mass fraction of water generally decreased from the entrance conditions (see Figure 11) due to the interaction of the cold droplets with the hot gas; consequently, the gas temperature also decreased (further addressed below). The droplet velocity decreased upon entry into the column; some of the droplets became entrained by the chaotic gas, recirculated within the chamber, and then finally exited through the chamber outlet leg.

The particle profiles shown in Figure 11 align with the gas-phase flow profiles presented in the preceding section (Section 5.1). The central jet stream, for all the models, is also visible in Figure 11. It is interesting to note that the central jet stream has particles with the lowest residence time. This is expected when one considers the high gas velocities in this stream, where the droplets move fairly fast in the column. The low residence times of the droplets in the central jet are accompanied by a high particle water mass fraction and larger droplet diameters. This is because the particles are not sufficiently exposed to the hot gas to result in appreciable drying, hence there is limited moisture reduction. The particle moisture content is reduced when moving radially toward the column wall, however a slight

increase is observed near the wall. The increase in moisture near the column wall agrees with the observed velocity profiles; for both the perfect shrinkage and classic d^2 law models, a velocity bias as a result of the flow deflection was observed toward the wall, particularly in the direction of the $-x$ axis—hence the apparent high moisture content, low residence time and larger diameter particles observed. On the other hand, the mechanistic model shows a relatively uniform and low moisture content of the recirculating particles in the column, except at the bottom conical section where high swirling (compared with that of other models) was observed. It is deduced that the particles swirl in the bottom conical section and decrease in size until they are sufficiently small to be entrained by the low-velocity air recirculating to the top of the column, hence the observed uniform and smaller particle sizes with correspondingly longer residence times and low moisture content occupy this section of the column. The temperature profiles generated for the different drying models are compared in Figure 12.

All the drying models accurately depict the high temperature zone immediately after the hot gas entry point into the column. The colder atomizing gas and generated droplet particles at the nozzle tip and subsequent travel down the column of this cold phase as part of the central jet is also evident from all the models. The different phases interact, resulting in the observed decrease in temperature of the heated gas, evident from the radial dissipation of heat in the midsection of the column. Regarding the heat dissipation within the column, the perfect shrinkage and classic d^2 law models have a shorter dissipation length from the top of the column due to the relatively higher velocity of the recirculating flow, which disrupts the central jet. The lower velocity in the mechanistic model therefore results in a longer dissipation length because of the undisturbed central jet. For both the perfect shrinkage and the classic d^2 law models, the previously highlighted bias of flow in the column toward one side is seen in the nonsymmetric temperature and humidity profiles in Figure 12.

The predicted humidity profiles of the continuous phase are shown in Figure 12. The simulations for all the drying models accurately predicted an increase in the gas humidity as the gas traverses down the column. The increase is as expected, as a result of the drying of the dispersed phase, with the evaporated moisture reporting to the gas phase. The central jet stream as initially presented in the single-phase results is also evident in the predicted humidity profiles. The high humidity associated with the central spray of droplets persists down the column until it impinges on the wall of the conical section of the scrubber. As a result of the recirculation of the air flow and the simultaneous entrainment of particles with a high mass fraction of water for the perfect shrinkage model and the classic d^2 law model as discussed previously in this same section, the humidity of the gas in this part of the column is preferentially higher. This bias is not seen for the mechanistic model, as expected, but the central spray protrudes further down the column to the conical section of the chamber where humidity increases because of the intense swirling in this region.

5.2.1. Spray-Drying Models: Validation. Validation of the drying models investigated in this work is now addressed. Two key parameters measured in the experiments were used in the model validation: temperature and moisture content of the product.

5.2.1.1. Comparison of the Drying Models Based on Temperature Prediction. The choice of spray drying model was based on the quality-of-fit of the model temperature (using both

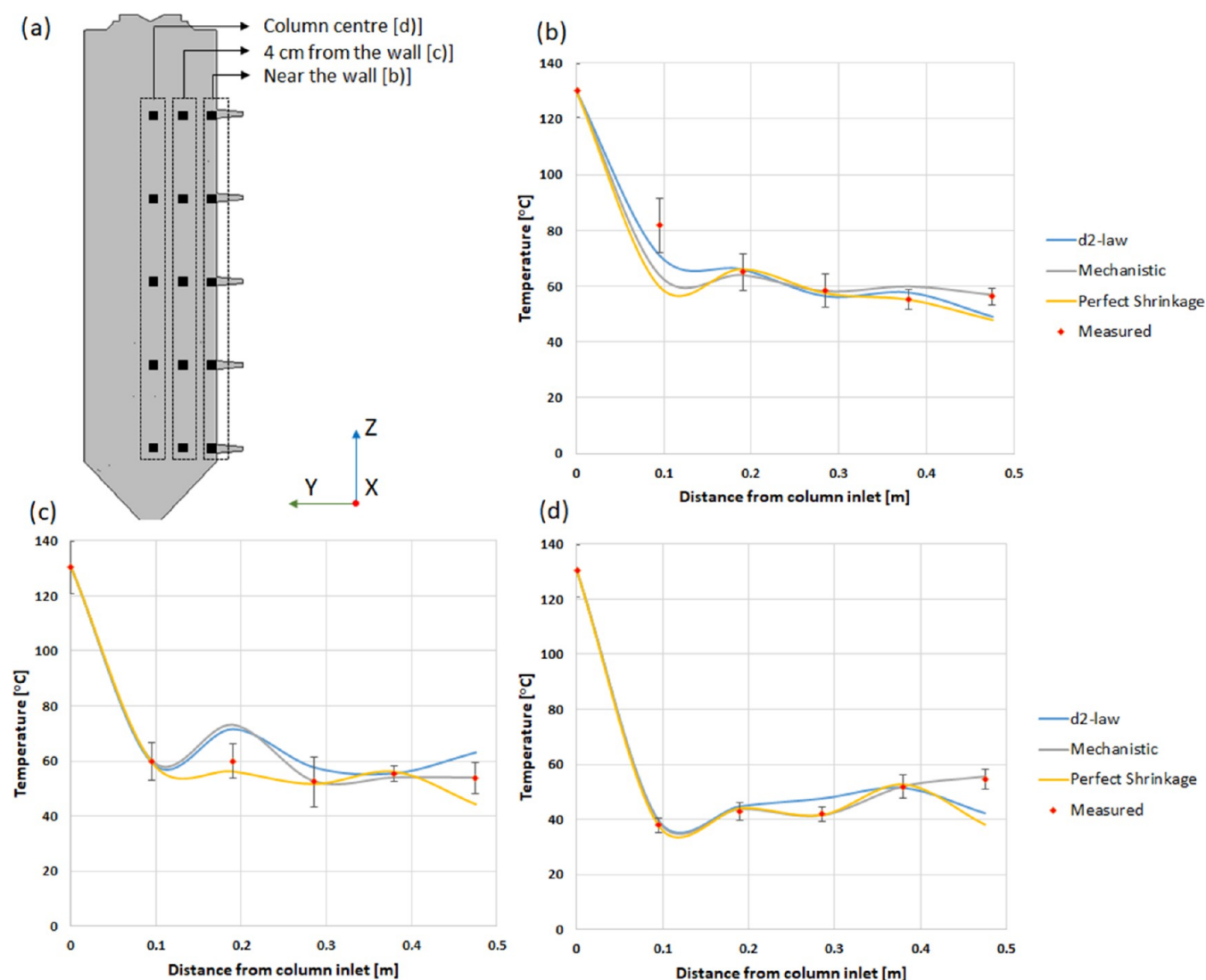


Figure 13. (a) Column y - z plane showing temperature measurement locations and temperature prediction plots of the different drying models along the column (where zero is the top of the column): (b) near the column wall, (c) 4 cm from the wall, and (d) at the column center. Comparison with experimental data is included.

Table 5. Quality-of-Fit of the Three Drying Models Compared with Experimental Data for Multiphase Flow Analysis

multiphase flow	flow within the chamber					flow exiting the chamber					
	quality-of-fit of temperature [°C]	distance from the wall				model T_{out} [°C]	measured T_{out} [°C]	% error - model T_{out}	model product moisture out [kg H ₂ O/kg material]	measured product moisture out [kg H ₂ O/kg material]	absolute difference in product moisture out [kg H ₂ O/kg material]
		near the wall	4 cm from wall	column center	overall RMSE						
perfect shrinkage	RMSE	9.0	4.0	6.3	6.7	53.7	55.7	3.6	0.024	0.032	0.008
classic d^2 law	RMSE	5.4	6.3	5.6	5.8	51.5	55.7	7.5	0.043	0.032	0.011
mechanistic	RMSE	6.9	5.1	0.8	5.0	56.7	55.7	1.8	0.038	0.032	0.006

the outlet temperature and the temperature profile within the column) compared with the experimental data. Figure 13 shows the temperature predictions of the different droplet drying kinetics models along the column at three points: (b) near the column wall, (c) 4 cm from the wall, and (d) at the column center.

Commencing with the general trend of the predicted temperatures, compared with the experimental values, all the

models accurately predicted the reduction in temperatures down the column for measurements both along the wall and at 4 cm from the wall. The models also accurately predicted the initial drop of the temperature at the center of the column, which is followed by a gradual increase toward the outlet. This observation is a result of having a cold slurry sprayed at the center of the column with hot air entering in the annular section. As the flow descends down the column, heat transfer between

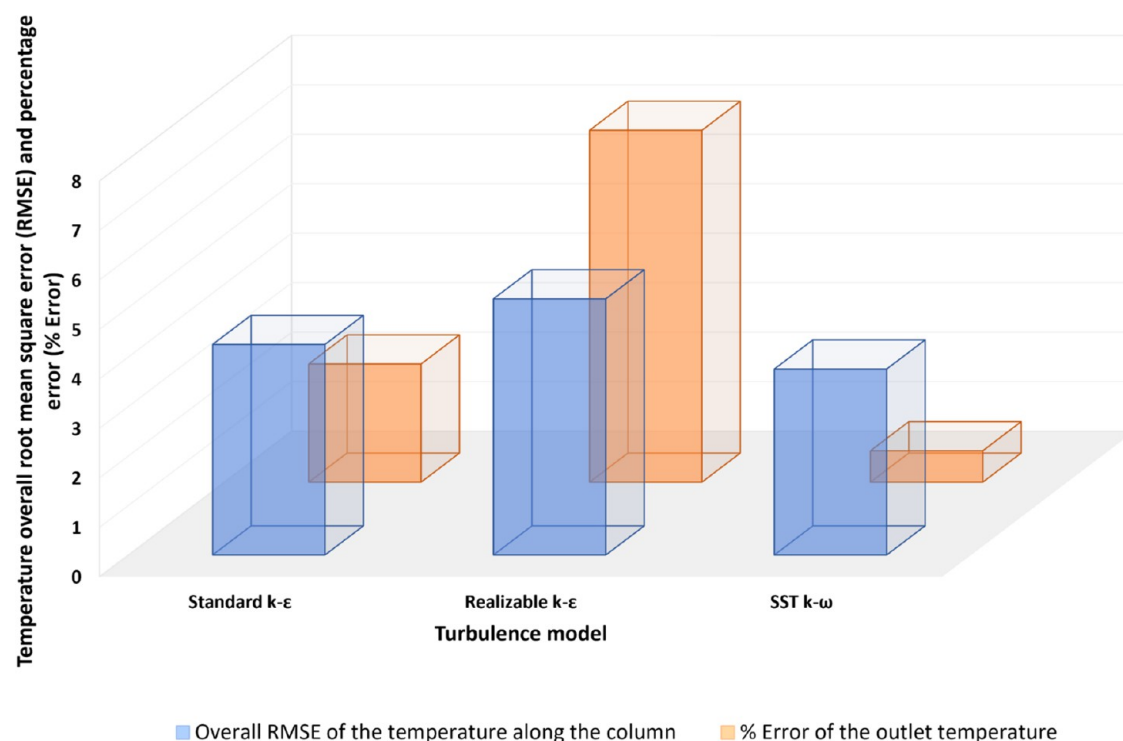


Figure 14. Comparison of the different drying models used for multiphase analysis.

the different streams takes place, resulting in a decrease in temperature of the outer 4 cm and wall sections and, simultaneously, gradually increasing the temperature of the air at the center of the column.

Table 5 and Figure 14 show the quality-of-fit of the investigated drying models to the experimental data. The best model was then deduced using the RMSE of the temperature within the column, the percentage error of the gas exiting the chamber, and the difference in the moisture content of the final product as predicted by the models and the experimentally determined values.

All the models generally overpredicted the temperatures inside the column, they also gave relatively similar RMSE values (Table 5) at the different radial positions across the column, except the mechanistic model, which, for the center and outlet temperature, generally gave good results. This may be attributed to the better mixing as previously shown in the velocity profiles for this model.

Table 5 includes the RMSE values for the three different drying models in terms of the overall temperature prediction inside the column. Results show that the mechanistic model gives better performance, followed by the d^2 law, and then the perfect shrinkage model (judged from the overall RMSE of the models). The better performance of the mechanistic model indicates that the effect of the presence of solids within the slurry droplets has an impact on the drying rate—a phenomenon for which the model is more suited. The temperature validation thus indicates that the best drying model for the dryer investigated in this work is the mechanistic model.

5.2.1.2. Comparison of the Drying Models Based on Moisture Removal Efficiency. A second approach used to confirm the best drying model for the spray dryer used in this work was validation using of the particle moisture content. The choice of the best drying model was made based on the absolute magnitude of the error between the experimental data and

model-predicted values. The lowest error in the predicted moisture was that noted for the mechanistic model, followed by the perfect shrinkage and last the classic d^2 law. Thus, in line with the earlier conclusion based on the RMSE of the temperature, the mechanistic model best describes the flow characteristics inside the chamber.

Observation of the model outlet temperatures together with the outlet average particle moisture content shows that a relationship exists between the two, where a high outlet average moisture content can be explained as being a result of less evaporation of water from the particles into the gas phase. This results in relatively high gas outlet temperatures as less energy is removed from the gas phase to provide the latent heat of vaporization. This is especially seen in the mechanistic model, which has the highest outlet temperature of the three drying models and a correspondingly higher average particle outlet moisture content. The behavior can be further explained from the theoretical derivation and basis of the mechanistic model which, unlike the other two models, considers the hindrance of the solids on the mass transfer rate, resulting in relatively lower evaporation rates. The lowest observed moisture content was in the perfect shrinkage model, which, contrastingly, does not have the lowest outlet gas temperature (as was expected). A possible explanation for this anomaly emerges from Figure 12, where some hot air is channeled toward the outlet leg due to the previously discussed flow bias, while a colder portion of the air recirculates to the top of the column. The lower temperature observed for the d^2 law model can be explained, in addition to the discussed flow bias, to a portion of colder air finding its way to the outlet leg, as (see Figure 12). Similarly, the slightly high particle outlet moisture observed for the d^2 law model can also be attributed to the channeling of air entraining bigger particles that have gone through limited drying in the column.

5.2.2. Effect of L/G on the Spray-Drying Process. The L/G is a parameter used to characterize the spray drying process and is

Table 6. Effect of L/G and Inlet Gas Temperature on the Spray-Drying Process for Five Different Cases Investigated in this Study

variables		Case 1	Case 2	Case 3	Case 4	Case 5	RMSE
inlet gas temperature [°C]		108.8	130.3	142.5	130.3	130.3	
L/G [kg/kg]		0.04	0.04	0.04	0.05	0.03	
inlet moisture content of the slurry [kgH ₂ O/kg material]		0.9	0.9	0.9	0.9	0.9	
outlet product moisture content [kgH ₂ O/kg material]	measured	0.180	0.032	0.017	0.055	0.017	0.034
	model	0.100	0.038	0.020	0.071	0.022	
outlet gas temperature [°C]	measured	47.1	55.7	71.8	53.0	63.0	3.0
	model	49.9	56.7	68.5	55.5	67.4	

considered as a critical parameter for scale-up purposes.⁴⁴ An increase in the inlet gas flow rate results in an increase in the available energy for the removal of water from the atomized droplets. However, the removal rate also depends on the particle residence time within the dryer, where an increase in the flow rate correspondingly leads to a decrease in the overall particle residence time.

The best models for spray-drying kinetics were determined to be the SST $k-\omega$ and mechanistic models (described in Sections 5.2 and 5.2.1). Having determined these, the CFD model was used to gain further insight into the effect of change in the L/G ratio. Table 6 presents the results for the five cases that were investigated where the effect of the L/G on scrubber operation was analyzed. In all cases considered here, an inlet slurry moisture content of 0.9 water mass fraction was used, and the model-predicted outlet temperature and moisture content were compared with experimental findings. For all the cases investigated, good agreement was obtained between the model-predicted and measured product moisture and outlet temperature as seen from the values of the RMSE. The calculated RMSE values for the moisture content and outlet temperature were 0.034 and 3, respectively.

Table 6 reveals that Cases 2, 4, and 5 have the same inlet temperature but different L/G ratios. Placed in the ascending order of the L/G ratio, the order becomes Case 5, Case 2, Case 4. The measured and model outlet moisture content increased with an increase in L/G ratio, as expected, since the available energy for mass transfer present in the incoming gas for the comparable liquid flow is reduced. The outlet temperature from the three cases for both measured and model-predicted results indicate that an increase in L/G results in a decrease in the outlet temperature. This is expected, given that an increase in L/G results in increased available water to gas in the system; this, in turn, leads to an increased energy demand for evaporation, thereby reducing the temperature of the gas. The internal column dynamics at the highest investigated L/G ratio (0.05) are shown in Figure 15 and corroborate the deductions.

It is evident from Figure 15 that there is clear recirculation of the gas toward the top of the column (as seen from the velocity profile), leading to increased radial heat dissipation as the gas interacts more intimately with the particles that have been entrained to the column top. The particle dynamics also show a dense particle presence at the top of the chamber, with high residence times and a low water mass fraction, indicating intense recirculation and heat exchange in this region of the chamber as the L/G ratio is increased. The particles reporting to the outlet leg (Figure 15b) indicate that the particles circulating at the bottom of the tower find their way through the outlet leg, hence there is a higher mass fraction of product reported in Table 6 compared to the lower L/G ratios. The temperature profile also shows a portion of warm gas reporting to the outlet leg, which

results in the increased outlet temperature, compared to the lower L/G ratio cases reported in Table 6.

5.2.3. Effect of Inlet Gas Temperature on the Spray-Drying Process. The effect of change in the inlet temperature on the process dynamics is evident from the results in Table 6, where we note that Cases 1–3 have the same L/G ratios but varying inlet temperatures. The measured and model-predicted average outlet moisture content, as expected, decrease with an increase in inlet temperature. This is due to the high driving force for evaporation at high temperatures resulting in a reduction of the particle moisture content. In terms of the effect of the inlet gas temperature on the outlet temperature, both the model and measured data indicated an increase in the outlet temperature resulting from an increasing inlet temperature. The additional energy entering with the inlet gas is used to remove the moisture from the particles, however, extra energy exits the system with the outlet gas. For all the energy to be utilized, the residence time of the particles within the chamber would have to also be increased, either by increasing the L/G ratio or introducing swirling in the atomization process. Figure 16 shows the case of a low inlet temperature (108 °C): Case 1 of Table 6.

In Figure 16, the velocity profile shows a slight bias of flow toward the side of the column ($-x$ direction). The biased stream entrains particles with a high moisture content (these particles also have a low residence time). The region is also associated with low gas temperatures. Notably, the temperature of the bulk of the gas is reduced as it contacts the cold droplets, and then exits the column at low temperatures (see Table 6). Although the gas leaves at a lower temperature compared to in cases with an increased inlet temperature, the low inlet gas temperature, and therefore the low heat duty of the gas, results in the droplets exiting the column with a high fraction of water. This was the case even though the associated particle residence time of the exiting particles was high, as is also evident from Table 6.

5.2.4. Dried Lime Product: Prediction of Particle Size Distribution. The model-generated particle size distribution (PDS) of the solid product was compared with experimental data. Results are shown in Figure 17, where a cumulative frequency distribution is presented.

The model results in Figure 17 are instantaneous results, collected after 10 s of Lagrangian injection flow time. A particle mean diameter (d_{50}) of 2.37 μm compared with 3.47 μm was obtained for the model and experimental data, respectively. Ninety percent of the particles were <3.80 μm for the model and 4.66 μm for the experimental measurements, while 10% of the particles were <1.4 and 2.48 μm for the model and experimental measurements, respectively. The distributions indicated that the model-predicted particles had sizes smaller than those measured in the laboratory, with the predicted distribution being to the left of the measured distribution. This could be due to agglomeration of particles within the dryer as well as during subsequent handling postsampling in a laboratory setting, which

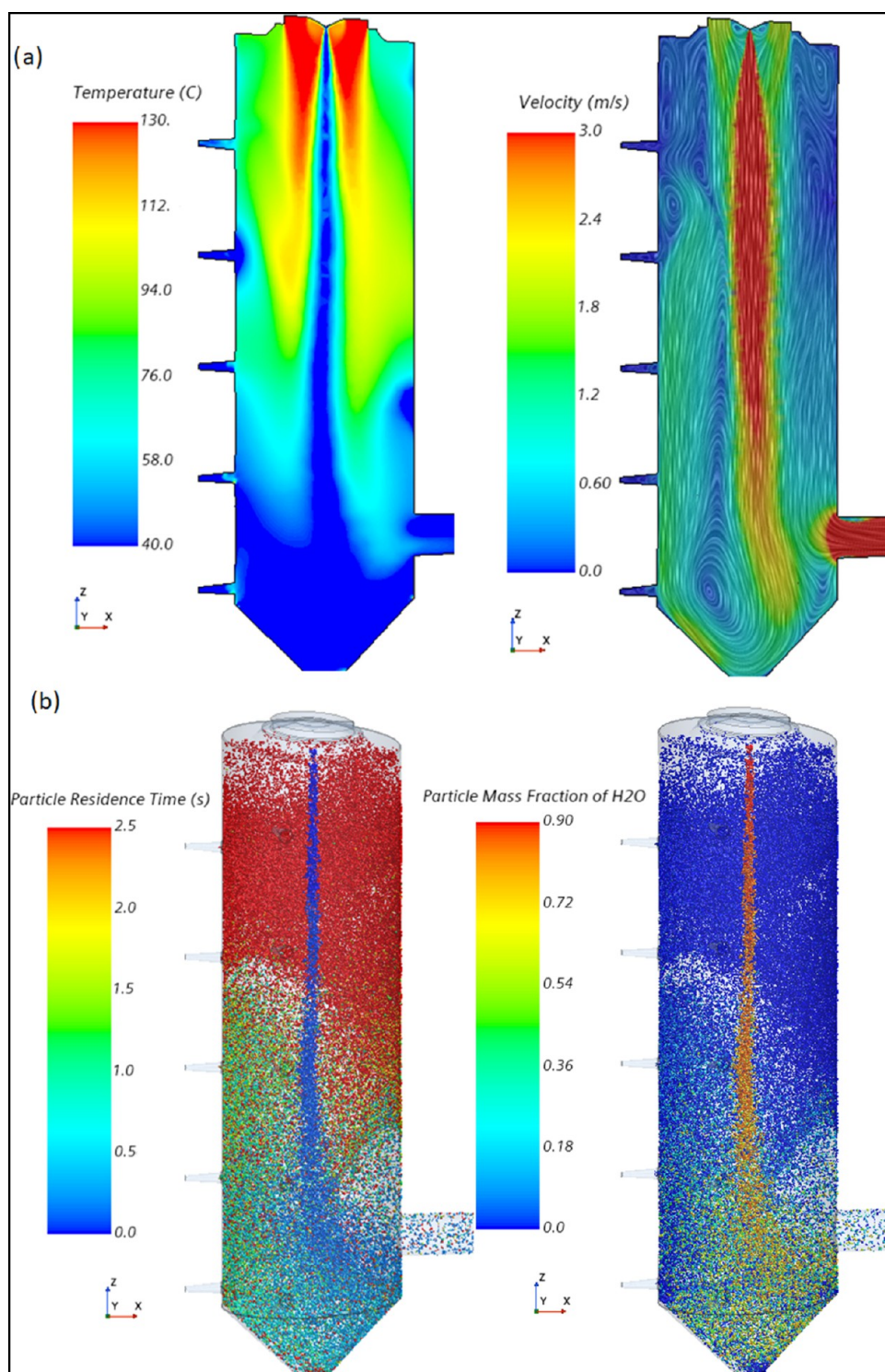


Figure 15. Comparison of the resultant (a) gas dynamics [temperature and velocity profiles] and (b) particle dynamics [Particle residence time and water mass fraction] along the x – z plane at the investigated L/G ratio of 0.05 (Case 4–Table 6) after 10 s of Lagrangian injection flow time.

was not accounted for in the modeling approach used in this work.^{45,46}

6. CONCLUSIONS

We have presented a detailed modeling approach for spray dry scrubbers, with particular focus on the BUCHI-B290 laboratory spray dryer. Detailed geometric representation of the dryer, heat loss to the environment, and inclusion of the downstream

cyclone impact on the chamber dynamics were implemented in the model. Results showed convoluted and chaotic flow behavior within the column. The choice of an applicable turbulence model was investigated via the single-phase flow case, where three two-parameter models were investigated for their ability to predict the flow behavior. The converged single-phase flow solution was then used as an initial estimate for the multiphase flow model output, where the Lagrangian phase was injected into the domain as a spray of droplets representing

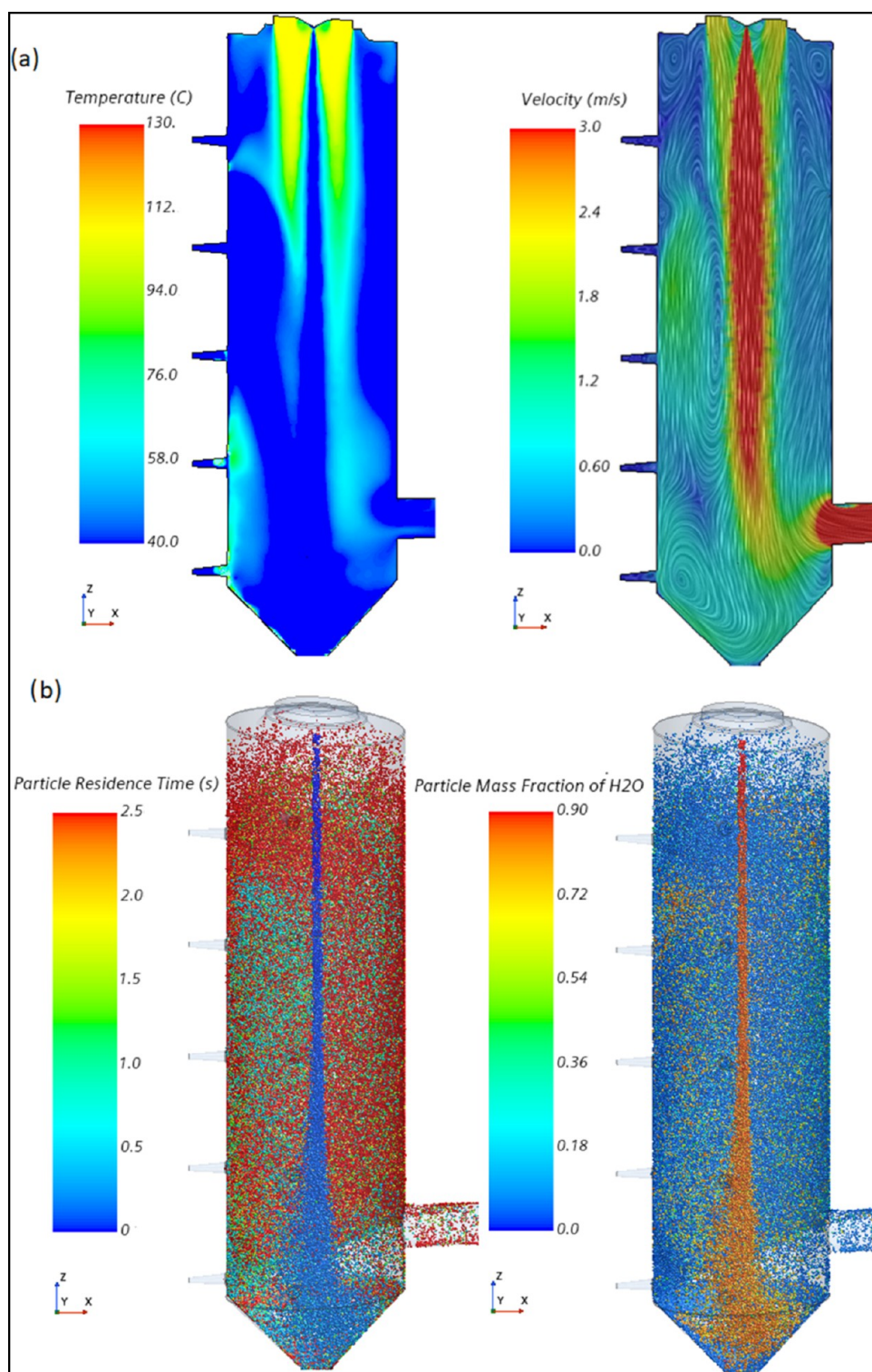


Figure 16. Comparison of the resultant (a) gas dynamics [temperature and velocity profiles] and (b) particle dynamics [Particle residence time and water mass fraction] along the x - z plane at the investigated inlet temperature of 108 °C (Case 1—Table 6) after 10 s of Lagrangian injection flow time.

the two-fluid nozzle used in the study. Three drying models, namely, the perfect shrinkage model, the classic d^2 law model and the mechanistic model, were also studied to determine the most suitable model for predicting droplet moisture removal and consequential gas flow dynamics. A study of the robustness of the applicable model in predicting process conditions was further addressed by investigating two critical dryer parameters, namely, the L/G ratio and inlet gas temperature.

The SST k - ω model was identified as the best model for adequate capture of the turbulence within the dryer. This was concluded after a thorough analysis of the flow field as well as a comparison of the model temperature predictions with experimental values. From the flow analysis, a central intact jet stream was observed, which was deflected as it impinged on the conical section of the dryer chamber, resulting in a chaotic recirculation and vortex formation as a result of the intense

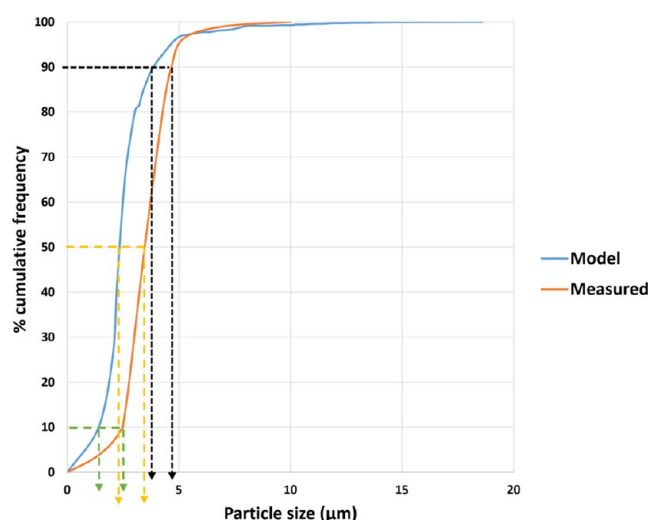


Figure 17. Comparison of the model-predicted lime solids product PSD with experimentally evaluated PSD (showing d_{90} , d_{50} , and d_{10} particle sizes) at 130.3 °C gas inlet temperature and 0.04 L/G ratio.

swirling of the flow field in the dryer. Subsequent analysis of the particle dynamics within the dryer showed some entrainment as the particles closely followed the gas flow pattern. The convoluted nature of the process and the impact of the drying model on the predicted column dynamics was evidenced by the different flow behaviors within the column, which resulted in different temperature profiles, humidity profiles and product moisture content associated with the different models.

The mechanistic model was found to give the best representation of the complex heat and mass transfer within the dryer, contrary to the assumption made in previous studies where the simpler perfect shrinkage and classic d^2 law models are generally assumed. This owes to the technical rigor of this model when compared with the other investigated models when dealing with droplets with suspended or dissolved solids as is the case in this study where lime slurry droplets were used. All models predicted a reduction in the gas temperature down the column and an associated increase in the humidity as well as a decrease in the droplet moisture content, as expected for a typical drying process.

The robustness of the model was tested by varying the inlet temperature and L/G ratio. An increase in the inlet temperature resulted in an increased outlet temperature for both experimental and model predictions and lower product moisture content. Increased particle residence time was necessary for adequate utilization of the available energy for complete moisture removal. Further analysis showed that an increase in the L/G ratio resulted in an increase in the outlet moisture content, as validated by experimental findings. The model accurately predicted a decrease in the outlet temperature with an increase in L/G.

The outlet PSD was also modeled. The model results showed a larger mean PSD (d_{50}) compared with experimental results, possibly attributed to the fact that the current model does not include droplet collision and particle breakage, which may have characterized the process dynamics.

In summary, we developed a comprehensive CFD spray drying model and a comparative study of different key models involving turbulence and droplet drying kinetics was carried out. Although these models have been utilized in various studies reported in literature, a broad comparative investigation with

detailed associated experimental undertakings, as carried out in this study, has not been reported to date (to the best of the authors' knowledge). The work further concludes that prior assumption of the models' applicability in drying applications may not be adequate, and where accuracy is of importance, conducting a comparative study must be undertaken provided resources permit. In the case where the computational cost is prohibitive, choosing the more complex hindered mechanistic model should be preferred. The work done in this study adds more insight into the water removal process achieved in spray dry scrubbing and indeed in any drying process.

The accuracy of the generated spray drying model developed in this work could be increased by including detailed chamber entrance dynamics, particle–particle interaction and more representative wall impingement modeling, the benefits of which should be weighed against the associated computational cost. In addition, other turbulence models capable of improved representation of the central jet may be investigated as well as investigating the impact of changing the scrubber velocities for the other drying models, as was done in the present study for the mechanistic model (by changing the L/G ratio). Further work to investigate other hindered drying models such as the lumped parameter and internal diffusion-based models is also recommended.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.iecr.4c02014>.

Additional information on the boundary conditions used in the study (PDF)

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Funding

This research was funded by Eskom Holdings SOC Limited grant numbers GT/WR2011.11.08. and 4600061784. The financial support and assistance received from the Eskom Power Engineering Programme (EPEP) and in particular, support provided to Letsabisa Lerotholi, a student at the EPEP Emissions Control Specialization Centre is acknowledged.

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

The authors are grateful for access to high computing power from the Centre for High Performance Computing national integrated cyber-infrastructure system (NICIS) supported by the Department of Science and Innovation (DSI), South Africa. The authors gratefully acknowledge the financial support and assistance received from the Eskom Power Engineering Programme (EPEP). In particular, the financial support provided to Letsabisa Lerotholi, a student at the EPEP Emissions Control Specialization Centre, North-West University (NWU), in collaboration with the Vaal University of Technology (VUT), is acknowledged. Special thanks go to Mr Preeya Sukdeo from Group Technology Engineering, Eskom Holdings SOC Ltd, for his input during the research.

NOMENCLATURE

ρ density (kg m^{-3})
 $\vec{u}$ velocity (m s^{-1})
 w species mass fraction (–)
 D mass diffusivity ($\text{m}^2 \text{s}^{-1}$)
 t time (s^{-1})
 Nu Nusselt number (–)
 E energy per unit mass (J kg^{-1})
 P pressure (Pa)
 p partial pressure (Pa)
 λ thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
 τ stress tensor (Pa)
 τ^R Reynolds stress tensor (Pa)
 T temperature (K)
 ω specific dissipation rate (s^{-1})
 k turbulent kinetic energy ($\text{m}^2 \text{s}^{-2}$)
 $\vec{x}$ position (m)
 d diameter (m)
 $\vec{v}$ particle velocity (m s^{-1})
 μ viscosity (Pa s)
 μ_t Eddy viscosity (Pa s)
 g gravitational term ($\text{m}^1 \text{s}^{-2}$)
 Re Reynolds number (–)
 Pr Prandtl number (–)
 Sh Sherwood number (–)

Sc Schmidt number (–)
 C_D coefficient of drag (–)
 C_p specific heat capacity (J K^{-1})
 h heat transfer coefficient ($\text{W m}^{-2} \text{K}^{-1}$)
 A area (m^2)
 h_{vap} latent heat of vaporization (J kg^{-1})
 $k_{i,g}$ gas-phase mass transfer coefficient for component i (m s^{-1})
 K_i overall mass transfer coefficient for component i (m s^{-1})
 $S_{d,dagg}$ geometric parameter (m)
 A_{agg} agglomerate area (m^2)
 ϵ tortuosity parameter (m)
 m molar flow rate (mol)

SUBSCRIPTS

A species A
 B species B
 d droplet
 p particle
 m mass
 s droplet/particle surface
 m momentum
 k k th particle
 g gas
 l liquid
 ∞ bulk phase
 E energy

SUPERSCRIPTS

$\cdot$ vector term
 $\cdot$ Rate

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