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Computer Aided Design for Spray Driers

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Abstract

The aim of this work is to develop an axi-symmetric two dimensional model based on a coupled simplified Computational Fluid Dynamic (CFD) and Lagrangian method to predict the air flow patterns and drying of particles. Then using this predictive tool to design more efficient spray dryers. The approach to this is to model what particles experience in the drying chamber with respect to air temperature and humidity. These histories can be obtained by combining the particles' trajectories with the air temperature / humidity pattern in the spray dryer.

Results are presented and discussed in terms of the air velocity, temperature, and humidity profiles within the chambers and compared for drying of a 42.5% solids solution in a spray chamber 2.22 m in diameter with a cylindrical top section 2.00 m high and a bottom cone section 1.725m high.

Keywords: drying, spray driers, computer aided design.

Introduction

Spray drying is a process for converting of a liquid feed into a powder by evaporation of the solvent. The basic principle of a spray drying process is the extensive contacting of the liquid with the drying medium, usually air. The air provides the energy for the evaporation and absorbs the solvent vapor (usually water). Four stages can be discerned in the spray drying process. The first stage takes place at the core of the process: the atomizer. The second stage is the dispersion of particles in the air and drying itself is considered the third stage. Collecting the powder is the last stage. Procedures for designing spray dryers are still very much up to individual, being based on practical experience and basic principles, and not on more theoretical approaches related to empirical methods and analytical/stepwise techniques. A single procedure can never be universally applicable since each variation in atomizer, air disperser, component design and location requires a separate mathematical model [1].

A spray-dryer designer often needs to predict behavior or performance of dryers before they are built. For that purpose, models are necessary. A good fundamental model of a spray drying process can only be constructed if we can devise both a good feedstock model and a good equipment model. If there are deficiencies in either, the overall model will be of strictly limited value [2]. The equipment model is a combination of factors that address the environment of a particle (e.g. air temperature, air humidity), while the set of factors that address the responses of a particle is called the feedstock model. The equipment model thus comprises the influence of the spray drying process on the quality of the product. Here, product quality consist of parameters such as moisture content, thermal degradation, aroma retention, shape and size of the particles and stickiness [3].

Several equipment models have been developed in the past decades [1]. Most of them are based on crude assumptions of what take place in the spray drying chamber, especially with respect to spray-air mixing. In most models, variations in air temperature and residence times are neglected; the flow of air and particles is not considered [4].

One of the big problems facing spray dryer designers is the complexity of spray/air mixing process in the spray chamber, then the difficulty in predicting particle

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trajectories within spray chamber. Because in the past it had not been possible to predict the aerodynamics of the spray chamber, designers have had to rely on their experience to avoid wall build and insufficient drying time problems. Computational fluid dynamics (CFD) technique, which predicts flow patterns and particle trajectories within the spray chamber on a more theoretical basis, has recently as a valuable tool to aid designers and investigate these problems [5].

In the CFD approach the spray –air mixing is addressed by combining airflow and particle trajectories, yielding temperature and humidity pattern in the spraying chamber, which in turn, when combined with the particle trajectories, results in the temperature and moisture content histories of the particles.

Mathematical Model

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The flow in a spray dryer is two-phase (air and droplets or air and particles). Hence, we employed an axisymmetric two dimensional fundamental model, in which the air phase is modeled as a continuum using the vorticity -stream function approach (simplified CFD). This approach was developed by Gosman [6] to model the fluid flow inside the pipes.

The air flow is governed by the mass, momentum, and energy conservation equations, these governing equations were formulated using vorticity and stream function as the dependent variables which reduce the number of equations by one and eliminate pressure as dependent variables.

The particle phase is modeled by the Lagrangian method, where the influence of droplets / particles on the air phase is considered as a source of mass and energy. These exchange terms were fed back to the airflow pattern calculation to obtain a two-way coupled solution. To calculate the exchange of mass and energy, the drying kinetics of the material had to be incorporated in the model.

A fundamental mathematical model of spray drying was solved at the following assumptions:

- 1. In the spraying, many particle fractions with various diameters and hence different drying times occur. Therefore, the droplet size distribution (DSD) is
- included in the formulating of the mathematical model.2. The droplets are spherical, and there is no temperature gradient inside the particle.
- 3. The complex mixing effects in the vicinity of the atomizer are neglected
- 4. Flow of the drying agent (air) is laminar and co-current.
- 5. The regular regime method of drying mechanism is used as the feedstock model. This method is based on the observation that the drying rate, after some time, will only depend on the actual moisture content and that the influence of the initial conditions decreases to virtually zero [7].

- 6. To predict histories of the droplets and changes of the temperature and humidity of the air within the spray dryer, we assume that for all droplets the initial droplet velocity is the same.
- 7. The main concept of the model consists in attribution to each particle some amount of ambient air. For such a system, a given amount of air-particle momentum, heat and mass balances are solved separately for each fraction. Since the feed rate is less than 10 % of the air mass flow rate, we can assume the momentum transfer from droplets to gas may not be significant [8].

Standard formulation of the differential equations

According to the above assumptions, the following equations are formulated as a general elliptical equation:

$$a_{\varphi}\left\{\frac{\partial}{\partial z}\left(\varphi\frac{\partial\psi}{\partial r}\right) - \frac{\partial}{\partial r}\left(\varphi\frac{\partial\psi}{\partial z}\right)\right\} - \frac{\partial}{\partial z}\left\{b_{\varphi}\frac{l_{2}r}{l_{1}}\frac{\partial(c_{\varphi}\varphi)}{\partial z}\right\} (1)$$
$$-\frac{\partial}{\partial r}\left\{b_{\varphi}\frac{l_{1}r}{l_{2}}\frac{\partial(c_{\varphi}\varphi)}{\partial r}\right\} + l_{1}l_{2}rd_{\varphi} = 0$$

The ϕ is taken as the dependent variable, and $a_{\phi}, b_{\phi}, c_{\phi}$ and d_{ϕ} are taken as standing for various function as represented in Table 1. Here the r is equivalent to l_3 .

Table 1 Functions associated with equation (1)

(0)	a.,	bo	Co	d_{φ}
C	1	Herr/Sc	1	$-(\Delta M_d/dV)$
T	1	Har /Pr	1	$-(\Delta E_d/C_{pa}.dV)$
rw	1	Harr.r2	$1/r^{2}$	0
W	0	$1/0.r^{2}$	1	-w/r
ω/r	r ²	r ²	Heff	$-\partial/\partial z (\rho.w^2)$

Droplet field calculations

The droplet field is established by integrating the differential equations for droplet motion to determine droplet velocities and, with further integration, droplet trajectories. At each time step along the trajectory, droplet size and temperature history are calculated using the equations for droplet mass and heat transfer rates.

The mass flow rate associated with droplet size (di) is given by:

$$\dot{m}_{d(di)} = \dot{m}_d \cdot y_i \tag{2}$$

Where \dot{m}_d is the droplet mass flow rate and y_i is the mass fraction associated with size d_i. The number flow rate along trajectory i is given by:

$$\dot{n}_i = \frac{\dot{m}_d y_i}{m_{(di)}} \tag{3}$$

Where $m_{(di)}$ is the mass of droplet with initial diameter of d_i . The number flow rate along a given trajectory is constant provided no coalescence or shattering occurs.

Momentum balance equations

A particle trajectory is calculated by integrating the equation of motion over time. This equation can be derived from a substitution of all forces working on the particle in Newton's second law [9].

$$m_{d} \frac{d\vec{U}}{dt} = \frac{C_{D}\rho_{a}A_{d} \left| \vec{V} - \vec{U} \right| \left(\vec{V} - \vec{U} \right)}{2}$$

$$+ \frac{\pi}{6} d^{3} (\rho_{d} - \rho_{a}) \vec{g} - \frac{\pi}{4} d^{3} \rho_{a} \nabla P$$

$$\tag{4}$$

The first term denotes the drag force of the air on the particle. The second term is the buoyancy force, and because the density of the particle is much larger than the air, this term constitutes the gravitational force. The last term is the pressure gradient force and is negligible in the case of spray drying. Therefore, the equation of motion for a droplet is given by:

$$m_d \frac{d\vec{U}}{dt} = \frac{C_D \rho_a A_d \left| \vec{V} - \vec{U} \right| \left(\vec{V} - \vec{U} \right)}{2} + m_d \vec{g}$$
(5)

Where:

$$f_{D} = \frac{C_{D}}{24} \operatorname{Re}, \operatorname{Re} = \frac{\rho_{d} |\vec{V} - \vec{U}|}{\mu_{eff}}, m_{d} = \frac{1}{6} \pi d^{3} \rho_{d}, A_{d} = \frac{1}{4} \pi d^{2}$$
$$\therefore \frac{d\vec{U}}{dt} = \frac{18 \mu_{eff} f_{D}}{\rho_{d} d^{2}} (\vec{V} - \vec{U}) + \vec{g}$$
(6)

$$\vec{U} = \vec{V} + \vec{g}\tau \left(1 - \exp\left(-\frac{\Delta t}{\tau}\right)\right) + \left(\vec{U}_0 - \vec{V}\right) \exp\left(-\frac{\Delta t}{\tau}\right)$$
(7)

Where dynamic characteristic time is defined by:

$$\tau = \frac{\rho_d d^2}{18\mu_{eff} f_D}$$

$$U_{Ax} = v + g\tau \left(1 - \exp\left(-\frac{\Delta t}{\tau}\right)\right) + \left(U_{Ax0} - v\right) \exp\left(-\frac{\Delta t}{\tau}\right)$$
(8)

$$U_{Rad} = u + (U_{Rad0} - u) \exp\left(-\frac{\Delta t}{\tau}\right)$$
(9)

After the new velocity is determined at time (Δt), the droplet position at the time (Δt) is determined from:

$$\frac{d\bar{x}_d}{dt} = \frac{\bar{U} + \bar{U}_0}{2} \tag{10}$$

$$\therefore \vec{x}_{d} = \vec{x}_{d0} + (\vec{U} + \vec{U}_{0}) \frac{\Delta t}{2}$$
(11)

$$x_{d,Ax} = x_{d,Ax0} + (U_{Ax} + U_{Ax0})\frac{\Delta t}{2}$$
(12)

$$x_{d,Rad} = x_{d,Rad0} + (U_{Rad} + U_{Rad0})\frac{\Delta t}{2}$$
(13)

Mass balance equations

To calculate an actual drying rate of a particle, a rigorous feedstock model which depends on a regular regime method is used [7].

Schoeber [10] discerned three stages in the drying curve by looking at the water concentration in the centre of the particle. These are the constant activity period, the penetration period, and the regular regime. The following equations for calculating the drying rate are employed:

In absence of penetration period

a. If X>X_c (constant activity period):

$$\frac{dm}{dt} = -KA\rho_a \left(c_{wl} - c_w \right) \tag{14}$$

Where K is the mass transfer coefficient, A is the area and it equals to πd^2 .

The interfacial water vapor mass fraction c_{wi} can be calculated using the vapor pressure, which is calculated from the Antoine relation [11]:

$$p_{vap} = p_{sat}(T) \cdot A_w(M_w)$$
(15)

 A_w (activity of water) is a function of M_w (moisture content), using a sorption isotherm curve of the material.

$$c_{w_i} = \frac{18p_{vap}}{29 - 11p_{vap}}$$
(16)

 p_{sot} as a function of wet bulb temperature T_{wb} was obtained by Antoine equation:

$$\ln p_{sat} = 16.2887 - \frac{3816.44}{T - 46.13} \tag{17}$$

and

$$K = \frac{Sh D_{eff}}{d}$$

The Ranz-Marshall correlation [12] for forced convection effects is used:

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$$Sh = 2.0 + 0.6Sc^{0.33} \operatorname{Re}^{0.5}$$
 (18)

$$\therefore \frac{dm}{dt} = -\pi Sh \rho_a D_{eff} d (c_{wi} - c_w)$$
⁽¹⁹⁾

b. If X<X_c (regular regime period): The flux is calculated as:

$$F = F_{PP}\left(T, X, X_{i}\right) \tag{20}$$

The flux parameter F is rendered into the mass flux:

$$\frac{dm}{dt} = -4\pi R^2_{2,0} \frac{1}{R_x} F$$
(21)

Where R_s is the solid shell thickness and is defined as:

$$R_{s} = \frac{R_{2,0} - R_{1,0}}{1 + X \frac{\rho_{s}}{\rho_{w}}}$$

In the present of penetration period

a. If X>X_c (constant activity period): Eq. 19 is applied
 b. If X_{s1}<X<X_c (penetration period): The flux is calculated using:

$$F = F_{RR}(T, X_{sl}, X_{l}) \frac{X_{0} - X_{sl}}{X_{0} - X}$$
(22)

The mass flux is calculated from Eq. 21.

c. If $X < X_{sl}$ (regular regime period): The flux is calculated as:

$$F = F_{PP}(T, X, X)$$

The flux parameter F is rendered into the mass flux as shown in Eq. 21.

Heat balance equations

Temperature of particles (drops) was calculated from the equation for drop side:

$$dq = hA(T_a - T_d) = m_d c p_d \frac{dT_d}{dt} - \frac{dm}{dt} \Delta H_{vap}$$
(23)

$$\therefore \frac{dT_d}{dt} = \frac{1}{m_d c p_d} \left[hA(T_a - T_d) + \frac{dm}{dt} \Delta H_{vap} \right]$$
(24)

where

$$\frac{dm}{dt} = -\pi Sh\rho_a D_{eff} d(c_{wi} - c_w) \text{ and } h = \frac{Nu k_a}{d}$$

Where

$$Nu = 2 + 0.6 \operatorname{Pr}^{.0.333} \operatorname{Re}^{0.5}$$
(25)
$$\therefore \frac{dT_d}{dt} = \frac{T_a - T_d}{\alpha} - \lambda \frac{(c_{wi} - c_w)}{\alpha}$$
(26)

where

$$\lambda = \frac{\Delta H_{vap} p Sh \rho_a D_{eff}}{N u k_a}, \qquad \alpha = \frac{\rho_d d^2 c p_d}{6 N u k_a}$$

$$T_d = T_{d0} + (T_w - T_{d0}) \frac{\Delta t / \alpha}{1 + \left(1 + \lambda \frac{d c_{w_i}}{d T_d}\right) \left(\frac{\Delta t}{2\alpha}\right)}$$
(27)

where

$$\frac{dc_{w_i}}{dT_d} = \frac{(18)(29)\frac{dp_{vap}}{dT_d}}{(29-11p_{vap})^2}$$
(28)

Droplet source term

The droplet source terms for the gas flow field are evaluated as the particles pass through the flow field. As a particle traverses a computational cell, it continually supplies mass and energy to the gas within the cell. Consider the trajectory shown in Fig. 1.



Fig.1 Decomposition of droplet path into series of continuous time steps

The number of particles associated with a time interval, Δt , is $\dot{n}\Delta t$ where n is the number flow rate along a given trajectory. The mass efflux due to these particles is:

$$S_{M} = \dot{n} \Delta t \left(\frac{dm}{dt}\right) \tag{29}$$

Summing overall time intervals associated with the particles traverse of the cell yields the net mass source term for that trajectory. Summing overall trajectories which traverse the cell yields the source term for that cell.

$$\Delta M_{d} = \sum_{iraj} \sum_{\Delta i} S_{M}$$
(30)

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Energy exchange between the gas and the droplet/particle arises through the convective heat transfer and the energy flux due to mass transfer. The energy source term, associated with time element Δt is given by:

$$S_{E} = \dot{n}\Delta t \left(\tilde{h}_{g} \frac{dm}{dt} - q_{d} \right)$$
(31)

$$\Delta E_{d} = \sum_{iraj} \sum_{\Delta i} S_{E}$$
(32)

where h_g is the enthalpy of the vapor leaving the droplet surface.

$$h_g = c p_v T_d \tag{33}$$

and

$$q_{d} = Nu k_{a} \pi d(T_{a} - T_{d})$$
(34)

Summing over time intervals and trajectories gives the energy source term for the cell.

Numerical Solution

In preceding section it was shown that a steady, laminar, two-dimensional flow is governed by the set of elliptic partial differential equations represented by the general Eq. 1 and the associated coefficients in Table 1; it is further controlled by the boundary conditions for all the variables along a surface which completely encloses the domain of interest. Thus, the problem of the prediction of two-dimensional flows has been reduced to a mathematical one; and solution of the equations will yield the distributions of the dependent variables ω, ψ, c_w, T , etc. throughout the flow.

Our task in the present section will be to derive a general solution procedure for the mathematical problem which we have posed. The solution procedure is a numerical one; and the main elements of its derivation are:

- 1. The confinement of attention to a finite array of points distributed throughout the flow as the nodal points of a grid.
- 2. The reduction of the differential equations to a set of simultaneous, algebraic finite difference equations, which relate the values of the variables at each node to the values which prevail at nearby nodes.
- 3. The recasting of the equations into a form suitable for solution by an iterative, successive-substitution technique.

A computer software is written in FORTRAN Power Station language and involving; input parameters, loops, subroutines, ...etc Fig. 2 shows the flow diagram of the computer program.



Fig. 2 Flowchart for sequence of operations in numerical model

Application of the model

One of the most detailed sets of the data available on the drying of a liquid feed spray issuing into a hot-air stream are those reported by Kieviet [12]. The spray dryer used in his experiments was a pilot-plant-scale cocurrent spray dryer (wide, squat body, diameter 2.2 m, height 3.725 m) manufactured by *Niro Atomizer*.

The drying air enters the drying chamber through an annulus; the nozzle is placed in the centre of the annulus.

The run selected with which to compare the model was that used an aqueous maltodextrin (Cerestar) solution. Maltodextrin is a carbohydrate mixture of high molecular weight and was used as a model compound because its material properties are well known and it is widely used in industry.

Results and Discussion

In Fig. 3 the modeled temperatures is depicted for the aqueous maltodextrin feed. In Fig. 3, the corresponding humidity pattern is depicted. From this figure it can be seen that a large volume of the dryer has almost constant temperatures and humidities. It appears that most of the drying takes place in the fast flowing core. The velocity of the airflow in the volume outside of the core is very low: it is almost stagnant. Further, particles appear not to be able to penetrate into this stagnant zone and are trapped in the fast flowing core. The Kieviet's measurements support the idea of a stagnant zone with hardly any temperature and humidity gradient.

Fig. 4 shows the predicted temperature profile and the measured data by Kieviet [12] at different levels in the drying chamber. We find that our predicted results agree well with the measured results.

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Fig. 3 Contour of modeled air temperatures and humidities distribution in the spray drying chamber (with spray). The predicted particle trajectories for the 4 particle sizes are depicted. Inlet air temperature =195 C, humidity =0.009, axial velocity v=9.0 m/s



Fig. 4 Comparison of temperatures and humidities at different levels measured from the ceiling (0.2, 0.6, 1.0 and 1.4 m) in the drying chamber between modeled results and measured results. The radial positions were 0.00, 0.29, 0.57, 0.85 and 1.11 m.

The simulation results provide details of the temperature field at different levels. From the predicted temperature profile, we find that the temperatures in the central core of radius of about 0.25m are different at different levels; this is expected as a direct result of drying. There is a minor radial variation in the air temperature. The largest temperature changes usually occur at the first level. It is a result of the very high heat and mass transfer rates in the nozzle zone due to high relative velocities between the gas and the droplets coupled with large temperature driving forces.

The predicted humidity profiles and the measured results of Kieviet [12] at different levels in the drying chamber are shown in Figure 4. We note that the predicted results and measured results in a broad slow flow region which it around the core, especially at the wall are different because of the nature of the flow where as it mentioned by Kieviel [12] was a slow circulation flow which leads to somewhat uniform distribution of humidity through this region. We find that the low humidity region and region of rapid change of humidity also occur in the central column. This implies that most of the drying takes place in this correregion. A large volume of the dryer chamber has almost constant humidity which means it is not used effectively for drying.

Conclusions

1. The varying chamber geometry and operatin parameters are likely to have significant effects on th flow patterns inside spray dryers. These changes wi affect the dryer performance, both in terms of produ moisture content and wall deposition rates.

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2. An interesting feature of this present model is that a fully coupling, axisymmetric two dimensional flow model is capable of simulation of gas-particle flow such as cyclone separator, liquid fuel combustors, fire suppression and pneumatic transport.

Nomenclature

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a _p	coefficient in the general elliptic Eq.1
Ad	droplet surface area (m ²)
A_{w}	water velocity (-)
b,	coefficient in the general elliptic Eq. 1
C _φ	coefficient in the general elliptic Eq. 1
Ср	specific heat (kJ/kg.K)
C _D	drag coefficient (-)
Cw	concentration of water vapor (kgw/kga)
d	droplet diameter (µm)
dø	source term in the general elliptic Eq. 1
Deff	diffusion coefficient (m ² /s)
D _{ch}	chamber diameter (m)
£	drag factor ()
JD Fpp	regular regime flux (kg/m s)
- AA	gravitational vector (m/s^2)
h	heat transfer coefficient $(k I/m^2 \circ K)$
ñ	antholmu (IsIA-)
k	thermal conductivity (k1/m a K)
K	mass transfer coefficient (m/s)
1	height of chamber (m)
l1, l2, l3	metric coefficients associated with coordinates
	z, r, and θ (-)
m	droplet mass (kg)
m _d	droplet mass flow rate (kg/s)
M	mass flow rate (kg/s)
M_w	moisture content (kg _w /kg _s)
n	number flow rate (l/s)
Nu	Nusselt number (-)
P Pr	Prandtl number ()
Ò,	heat transfer rate to droplet (kJ/s)
r	distance of a point from the symmetry axis (m)
R_{1}, R_{2}	radius of air bubble and radius of particle (m)
R _s	solid shell thickness
Re	Reynolds number (-)
SM	mass efflux (kg/s)
Se	energy ettlux (kJ/s)
Sh	Sherwood number (-)
t	time (s)
Т	temperature (K)

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U	velocity vector of droplet (m/s)
u	radial velocity of air (m/s)
V	volume (m ³)
v	axial velocity of air (m/s)
\vec{V}	velocity vector of air (m/s)
W	tangential velocity of air (m/s)
X	moisture (kg _w /kg _s)
Yi	mass fraction assigned to droplet size, di (-)
ΔH_{vap}	heat of evaporation (kJ/kg)
ΔM_d	mass source term due to droplets (kg/s)
ΔE_d	energy source term due to droplet (kJ/s)
μ_{eff}	effective viscosity of the fluid (kg/m.s)
ρ	density (kg/m ³)
φ	dependent variable of the general ellipatic Eq.
Ψ	stream function (kg/m.s)
ω	vorticity of the air (l/s)
θ	spray angle (°)
τ	dynamic characteristic time (s)
Subscr	ipts
a	air

a	air
С	critical
d	droplet
е	equilibrium
f	finished
i	interface
1	liquid
RR	regular regime
S	solid
sl	slurry
sat	saturation
v	vapor
W	water
wb	wet bulb
wl	wall

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