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Original article

Application of computational fluid dynamics to spray drying

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Abstract – In the computational fluid dynamics (CFD) analysis of spray dryers, the Euler-Lagrange model is used to compute the motions of the spray droplets and the heat and mass transfers between the droplets and the air stream. Such calculations are performed for hundreds to tens of thousands of droplets to represent the spray in the dryer. One limiting factor in drying mass transfer is the internal diffusion of water moisture inside partially dried particles. In order to model this internal diffusion of water moisture, each particle is represented by a series of concentric spherical shells. A one-dimensional diffusion equation is solved over these shells to obtain the internal distribution and diffusion of water moisture inside each particle. A key strength of CFD is the ability to carry out what-if and optimization analyses quickly. As an example, a dryer with a given set of feed conditions was considered. CFD simulations were carried out with the aim to find the optimum condition for the drying air. Key information of interest to the plant operator were extracted from the CFD results and presented in percentages of particles leaving the particle and air exits, and the particle conditions at these exits in terms of mean diameter, temperature and moisture content. From these results, the operator of the dryer can easily select the optimum operating conditions, which allows him to achieve the desired product quality at minimum cost.

spray drying / simulation / computational fluid dynamics

Résumé – Application de la dynamique des fluides calculée par ordinateur (CFD) au séchage par atomisation. Dans l'analyse de la dynamique des fluides dans les tours de séchage par atomisation, le modèle d'Euler-Lagrange est utilisé pour calculer les déplacements des gouttelettes et les transferts de chaleur et de masse entre les gouttelettes et le flux d'air. Ces calculs sont réalisés pour des centaines à des dizaines de milliers de gouttelettes pour représenter la pulvérisation dans la tour de séchage. Un facteur limitant dans le transfert de masse au cours du séchage est la diffusion interne d'eau à l'intérieur des particules partiellement séchées. Pour modéliser cette diffusion interne d'eau, chaque particule est représentée par une série de coquilles sphériques concentriques. La résolution d'une équation de diffusion mono-dimensionnelle sur ces sphères permet d'obtenir la distribution et la diffusion interne d'eau dans chaque particule. Un atout majeur de la CFD réside dans la possiblité de mener rapidement des analyses d'évaluation et d'optimisation. Par exemple, un équipement de séchage avec un jeu donné de paramètres d'alimentation a été étudié. Les simulations CFD ont été réalisées dans le but de déterminer les conditions optimales pour l'air de séchage. Les informations-clés d'intérêt pour l'opérateur ont été extraites des résultats de CFD et présentées en pourcentages de particules quittant les sorties, et les caractéristiques des particules à ces sorties en termes de diamètre moyen, de température et de teneur en humidité. A partir de ces résultats, l'opérateur de la

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tour de séchage peut aisément sélectionner les conditions opératoires optimales lui permettant d'obtenir la qualité désirée du produit au moindre coût.

séchage par atomisation / modélisation / dynamique des fluides

1. INTRODUCTION

Applications of computational fluid dynamics (CFD) techniques in analyses of spray dryers have been carried out successfully and reported by Straatsma et al. [5], Oakley et al. [4] and others. Most of these earlier works assume the flows in the dryers are two-dimensional and axisymmetric in order to reduce the demand on computational resources. The DrySim CFD software developed by Straatsma et al. [5] is an excellent example of these two-dimensional simulation tools.

In collaboration with Straatsma et al. at Nizo food research, we have integrated the DrySim model into a commercial CFD software, STAR-CD, so that we can apply the same modelling technology to fully three-dimensional geometries. In this paper, we will present some details of the mathematical model used and examine some of the results obtained from the CFD simulations.

2. MATHEMATICAL MODEL

The modelling technique used is generally referred as the Euler-Lagrange method, in which the conservation equations for mass, momentum and energy for the gas flow in the dryer are expressed in the Eulerian form and the droplets in the Lagrangian form. The complete description of these governing equations and equations representing the interactions between the two phases via drag forces, heat and mass transfers and turbulence can be found in the STAR-CD Methodology Manual [2].

For spray drying applications, the drying model is of critical importance. Therefore we will examine some details of the drying model below.

2.1. Internal diffusion of moisture

The external transport phenomena (from particle surface to surrounding air) and the internal transport phenomena (with the particles) both play an important role in the drying process.

Following Crank [3], the diffusion of moisture within a droplet is expressed by:

$$\frac{\partial c}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\frac{\partial c}{\partial r}\right) \qquad (1)$$

where r is the radial coordinate, c is the moisture concentration (kg·m^{-3}), and D is the diffusion coefficient (m^2·s^{-1}).

2.2. Water diffusion coefficient

The diffusion coefficient is strongly dependent on the local moisture content and temperature. According to Straatsma et al. [5] for dairy powders the following equations can be use to describe the diffusion coefficient (D) as a function of moisture content (W) and temperature (T):

$$\ln(D_W) = a_{1,T} - \frac{b_{1,T}}{c_{1,T} + W} \qquad (2)$$

and

$$\ln(D_T) = a_{2,W} + \frac{b_{2,W}}{T} \qquad (3)$$

where a_1, b_1, c_1, a_2 and b_2 are product specific model constants.

2.3. External mass transfer

The rate of evaporation at the droplet surface depends on the partial water pressure in the droplet surroundings and the partial water pressure at the droplet surface.

The rate of mass transfer ($\mathrm{kg{\cdot}s^{-1}}$) is therefore:

$$\dot{m} = \gamma A \frac{\tilde{M}_w}{\tilde{R}} \left(\frac{P_{w,\,s}}{T_d} - \frac{P_{w,\,\infty}}{T_\infty} \right) \quad (4)$$

where γ is the mass transfer coefficient, $A = \pi d^2$ is the surface area of the droplet, $\tilde{R}$ is the universal gas constant, $\tilde{M}_w$ is the molecular weight of water, $P_{w,\,s}$ is the partial pressure of the water vapour in equilibrium with the powder, $P_{w,\,\infty}$ is the water vapour partial pressure in the free-stream, T_d is the temperature of the droplet and T_∞ is the gas temperature in the free-stream.

2.4. Sorption isotherms

The partial water pressure at the droplet surface is related to the surface moisture content and the droplet temperature by sorption isotherms. For dairy products (and other food products), the GAB (Guggenheim, Anderson, de Boer) equation is widely used [5]:

$$W = W_m \cdot \left(\frac{(c_g - 1) \cdot K \cdot a_w}{1 + (c_g - 1) \cdot K \cdot a_w} + \frac{K \cdot a_w}{1 - K \cdot a_w} \right) \quad (5)$$

where a_w is the water activity, W the powder moisture content and W_m, c_g and K product specific constants. These constants can be temperature dependent.

2.5. Partial water vapour pressure at droplet surface

Water activity is the ratio of the partial pressure of water vapour in equilibrium with the powder ($P_{w,\,s}$) to the vapour pressure of pure water at the same temperature (P_{wa}). Hence,

$$P_{w,\,s} = a_w P_{wa}. \quad (6)$$

2.6. Partial water vapour pressure in the free-stream

The partial water vapour pressure in the free-stream is based on the moisture content of the air, x_a, expressed as *kg_water/kg_dry air*:

$$x_a = \frac{x_m}{1 - x_m} \quad (7)$$

where x_m is the moisture content based on the total mass (*kg_water/kg_water+air*). The water vapour partial pressure in the free-stream is therefore given by:

$$P_{w,\,\infty} = \frac{x_a P_t}{\frac{\tilde{M}_w}{\tilde{M}_a} + x_a} \quad (8)$$

where $\tilde{M}_a$ is the molecular weight of air and P_t is the total pressure.

2.7. Heat and mass transfer coefficients

The heat transfer coefficient, h, is given by Ranz-Marshall correlation for a sphere,

$$Nu = \frac{hd}{k} = 2 + 0.6\mathrm{Re}^{1/2}\mathrm{Pr}^{1/3} \quad (9)$$

where Nu is the Nusselt number, d is the particle diameter, k is the thermal conductivity of the gas phase. The droplet Reynolds number is given by:

$$\mathrm{Re} = \frac{\rho \left| u_d - u \right| d}{\mu} \quad (10)$$

and the Prandtl number by:

$$\mathrm{Pr} = \frac{\mu C_p}{k} \quad (11)$$

where ρ is the density, C_p is the heat capacity and μ is the viscosity of the gas phase. u_d and u are the velocities of the droplet and the gas, respectively.

The mass transfer coefficient, γ, is found from the equivalent correlation:

$$Sh = \frac{\gamma d}{D_{AB}} = 2 + 0.6\mathrm{Re}^{1/2}\, Sc^{1/3} \quad (12)$$

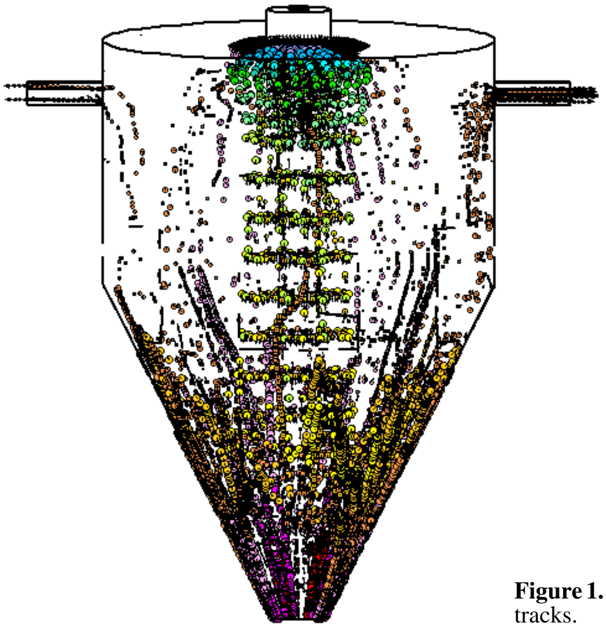

Figure 1. Spray dryer with computed particle tracks.

where Sh is the Sherwood number, D_{AB} is the diffusivity of water in air. The Schmidt number is given by:

$$Sc = \frac{\mu}{\rho D_{AB}}. \tag{13}$$

3. CFD ANALYSIS AND RESULTS

3.1. CFD analysis

In every CFD analysis, it is necessary to go through several steps to build the computational model, carry out the computation and analysing the results as follows:

(1) Define the shape and dimensions of the dryer.

(2) Specify the inlet and outlet configurations.

(3) Define the atomiser and the spray characteristics.

(4) Specify the flow rates of feed and drying air.

(5) Build a computational mesh.

(6) Run the solver to obtain a converged solution.

(7) Analyse the solution and produce a performance report of the dryer.

This sequence of steps together with the model equations described above provide us a well defined methodology in applying CFD in spray drying analyses. This methodology has been encapsulated, with the steps defined above automated, in a CFD software called “es-spraydry” [1] where “es” stands for expert-system tool.

3.2. Case study

We have a simple dryer shown in Figure 1. The outer diameter of the dryer is 9.5 m and an overall height of 14 m. There are one central air inlet and four circular air outlets. A rotary wheel atomiser spinning at 2600 rpm is used for the atomisation of the feed. The droplets produced are assumed to have a log-normal size distribution and a mean diameter of 100 µm with a geometric standard deviation of 0.6.

Table I. Summary of model data.

Material processed = milk powder
Dry solid density at 20 °C = 1542 kg·m^{-3}
Water diffusion coefficients according to equation (2)
At $T = 283$ K, $a_l = -22.64$, $b_l = 0.8962$, $c_l = 0.03981$
At $T = 343$ K, $a_l = -20.95$, $b_l = 0.6721$, $c_l = 0.05679$
Sorption isotherm, GAB coefficients according to equation (5)
$W_m = 0.059$, $c_g = 11.4$, $K = 1$

The dryer is required to process a feed at a rate of 4990 kg·h^{-1}, a temperature of 25 °C and a solid content of 55% w/w. Drying air is to be supplied at 185 °C with a moisture content of 1% w/w. We need to find the optimum air flow rate which will satisfy the following requirements:

(1) 90% of particles exit the bottom particle exit.

(2) Mean particle moisture content is less than 9% w/w.

(3) Mean particle temperature is less than 100 °C.

A summary of the model data used in the simulations is provided in Table I. From the CFD results we monitored the particle conditions exiting the dryer at the particle and air exits. Several CFD calculations were performed with different air flow rates, the results are summarized in Table II.

The results were further analyzed against the operation requirements graphically in Figures 2 to 4. The range of air flow rates which satisfy the requirements are listed in Table III. From the analysis we would select to use an air flow rate of 55 000 kg·h^{-1} for minimum operating cost, in terms of cost in supplying the drying air.

3.3. Computational details

The CFD model used in the analysis has 20902 cells, 100 parcels of droplets were used to represent the spray. Converged solutions for all cases were obtained within 200 iterations. The CPU times for the cases range from 4000 to 7555 s on an Intel P3, 1.2 GHz computer.

4. CONCLUSION

In this paper we reviewed the details of the drying model incorporated into the CFD calculations. The drying model includes a transport equation for the internal diffusion of the water moisture inside each particle.

Table II. Particle conditions at exits.

Air flow	Particle Exit				Air Exit			
kg·h^{-1}	%	diameter (μm)	Temperature (°C)	Moisture (% w/w)	%	diameter (μm)	temperature (°C)	Moisture (% w/w)
45 000	87.1	125	72.7	12	12.9	72.3	100	3.3
50 000	87.1	126.2	83.2	11	12.9	63.7	103.8	2.3
53 000	90	124	87	10	10	65	104	3
55 000	91.5	120	90.4	9.1	8.5	86.2	107	3
60 000	88.7	122.8	96.3	9	11.3	76.6	113.1	2.2
63 000	90.5	120	101	8.1	9.5	88.9	116	2.5
65 000	88.8	122.6	102.3	8.9	11.2	78.7	117	1.9
70 000	76.3	125.6	105	8.6	23.7	90.2	121	2.2

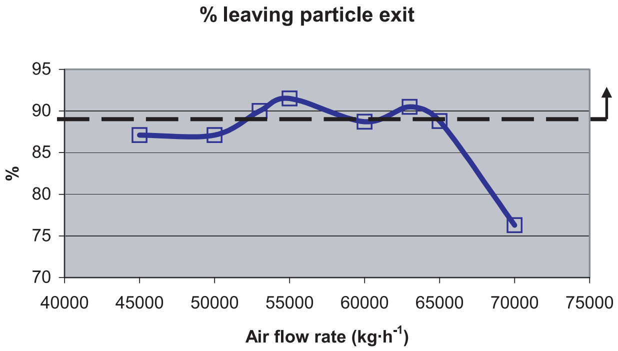

Figure 2. Percentage of particles leaving dryer at particle exit.

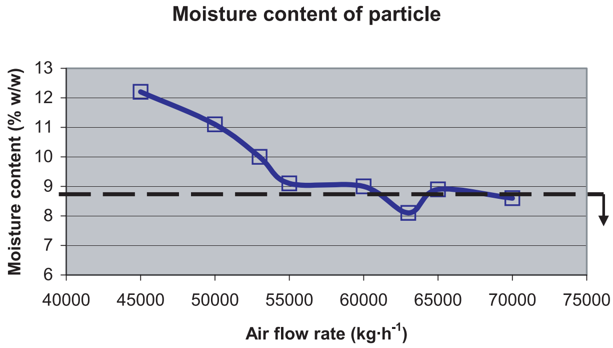

Figure 3. Average moisture content of particles leaving particle exit.

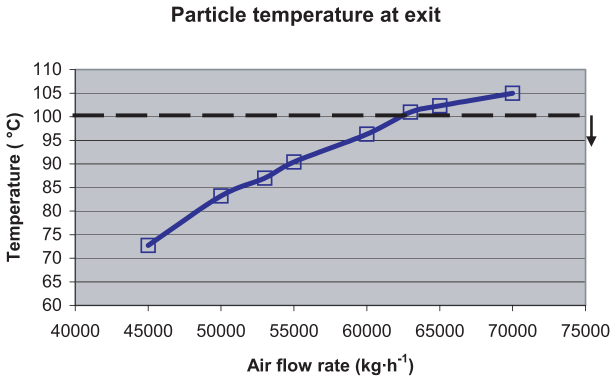

Figure 4. Average temperature of particles leaving particle exit.

Table III. Determination of air flow rate satisfy operation requirement.

Requirement	Air flow rate ($kg{\cdot}h^{-1}$)	Plot
(1) 90% of particles exit the bottom particle exit	53 000 – 65 000	Fig. 2.
(2) Mean particle moisture content less than 0.09	Greater than 55 000	Fig. 3.
(3) Mean particle temperature less than 100 °C	Less than 63 000	Fig. 4.
Satisfy all 3 conditions.	55 000 – 63 000	

Equations for the diffusion coefficient and sorption isotherm appropriate for daily products were described.

A simple case study was used to illustrate the ability of CFD in performing optimization analysis. The optimum air flow rate was determined for a given set of operating conditions and quality requirements for the powder product. From the analysis we obtained the range of air flow rate which would satisfy the operational requirements. We then selected the minimum air flow rate from this range so that the product can be produced at minimum cost.

Dedicated CFD software for spray dryer analysis, such as es-spraydry, have simplified and automated the process of CFD analysis. With these simulation tools it is now possible for the spray dryer operators to carry out systemic analysis of their dryers and to ensure their dryers are operating at optimum conditions.

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