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Mathematical Modeling of an Aqueous Film Coating Process in a Bohle Lab-Coater, Part 1: Development of the Model

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ABSTRACT

The purpose of this study was to develop a model to predict (1) air and product temperatures, (2) product moisture, and (3) air humidity during an aqueous coating process using a Bohle Lab-Coater. Because of the geometrical properties and the airflow, the drum of the Bohle Lab-Coater can in principle be divided into 2 zones of equal size—the drying and the spraying zones. For each zone, 4 balance equations could be set up describing the change of the air humidity, the product moisture, the enthalpy of the air, and the enthalpy of the product in each zone. For this purpose, knowledge regarding heat and mass transfer and also the motion of the tablets in drums was used. Based on the considerations of the heat and mass transfer, a set of first-order coupled ordinary differential equations (ODEs) was developed. This set of ODEs can be solved numerically. In this part, the development of the model is described in detail, whereas the application of the model can be found in part 2.

KEYWORDS: film coating, mathematical modeling, heat and mass transfer, convection, particle movement.

INTRODUCTION

Aqueous film coating is widely used within the pharmaceutical industry to apply either protection or functional coatings on tablets. Especially for functional coatings, smooth and homogeneous films are necessary to ensure the desired functionality. Several film-coating defects can occur as a result of improper drying conditions. Primarily cratering and sticking lead to defects that might be attributed to insufficient drying conditions. If the drying conditions are excessive, blistering or pinholes in the coating film might be observed.[1] In addition, insufficient drying conditions can lead to a decomposition of the active substance. This decomposition is usually a result of high temperature or high water content in the core. These undesirable effects display the necessity of optimizing the drying process. In different studies, the influence of inlet air temperature and humidity, air-flow rate, and spray rate on the quality of the product were investigated.

In many cases, designs of experiments were used to estimate the drying conditions. Franz and Doonan[2] used the surface temperature of the tablet bed measured by an infrared thermometer to predict the influence of spray rate, inlet air-flow temperature, and air-flow rate on the drying effect. Between atomizing air pressure or pan speed and the surface tablet bed temperature, a correlation could not be observed.[2] Because temperature alone is not a good indicator for the drying conditions, some authors used other parameters for the description of drying conditions (eg, the water removal efficiency[3] or the vaporization efficiency[4]). In both cases, the following mass balance for the calculation of the efficiency was used: during steady state, the input of water is equal to the removed amount of water. The input of water could be calculated from the spray rate and the water content of the coating preparation. The removed amount of water per time could be determined from the difference in the absolute air humidity of inlet and exhaust air, the air-flow rate, and the density of the air.[3] In both cases the influence of different process parameters on the vaporization efficiency/water removal was investigated to define an upper limit for the efficiency. Another possible way to estimate the drying conditions is with the Mollier-*h*, *x*-diagram.[5]

Film coating is generally expected to be an adiabatic process, where the complete enthalpy of the system remains constant. Ebey[6] used the first law of thermodynamics to derive equations that relate the drying rate during film coating and the process variable. This rate demonstrated the ratio of the area of the heat to the mass transfer under certain process conditions. He postulated that drying conditions with the same film-drying rate during the coating will lead to film tablets with the same conditions.

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The aim of this project was to develop a physical model for the prediction of air and product temperatures, product moisture, and air humidity in the Bohle Lab-Coater. Because the different temperatures, moisture, and humidity are time dependent, the model should not only describe the steady state.

MATERIALS AND METHODS

Depiction of the Process

The process that should be specified by a physical model is the coating of tablets with aqueous polymeric dispersions in a Bohle Lab-Coater. When spraying the dispersion onto the tablets, the water should be removed, so that a homogeneous film can be formed. The drying is performed using heated inlet air that flows through the tablet bed. For the modeling purpose, it is assumed that the heat and mass transfer mainly occurs by convection. In the following sections, the process is described with respect to some special constructive features of the coater.

The drum of the coater is evenly perforated and rotates during the coating process with a constant velocity of the circumference. The pan speed of the drum, which is directly related to the velocity of the circumference, should be chosen depending on tablet shape and size, so that a turnover of the tablets is possible. Besides the movement of the tablets in the direction of the revolution, a horizontal transport takes place. Therefore the drum has 2 inner and 3 outer mixing ribbons. Figure 1 shows the 3-dimensional placement of the mixing ribbons.

Figure 1. Coating drum with mixing ribbons.

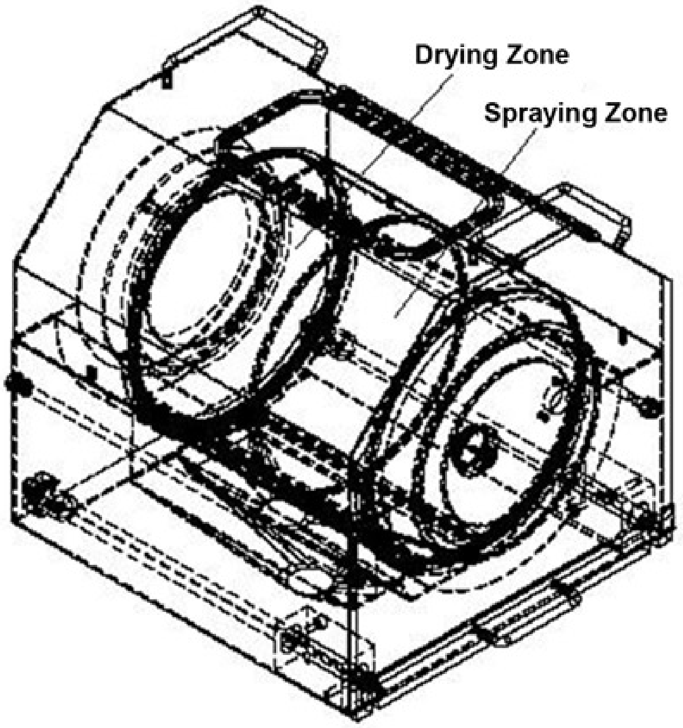

Figure 2. Schematic graph of the coating drum and the cabinet of the Bohle Lab-Coater.

Outside the drum there is a cabinet for the drying air. This cabinet is divided into 2 chambers that are connected via the perforation with the inside of the drum (see Figure 2). A short circuit between both chambers is impossible. Because of the position of the partition wall between the chambers, the drum can in principle be divided in 2 zones of equal size. In zone 1, the spraying zone, the tablets were coated and dried with the air flow coming from zone 2. In zone 2, the drying zone, the tablets were further dried by the heated inlet air that entered the drum from the bottom. The air flow goes from zone 2 to 1 before the air leaves the drum below the tablet bed. The movement of the tablets in the drum is performed by the mixing ribbons and by the inclination of the axis of rotation. During the coating process, different heat and mass transfers occur. They are shown in Figure 3 and are described by balance equations in the next section.

RESULTS AND DISCUSSION

Balance Equations of the Model

Due to the description of the process a two compartment model is suggested (Figure 3). Every zone is assumed to be ideal mixed. Based on that, zone balance equations could be set up for the moisture of the tablets, for the air humidity and for the enthalpy of the tablets and the air.

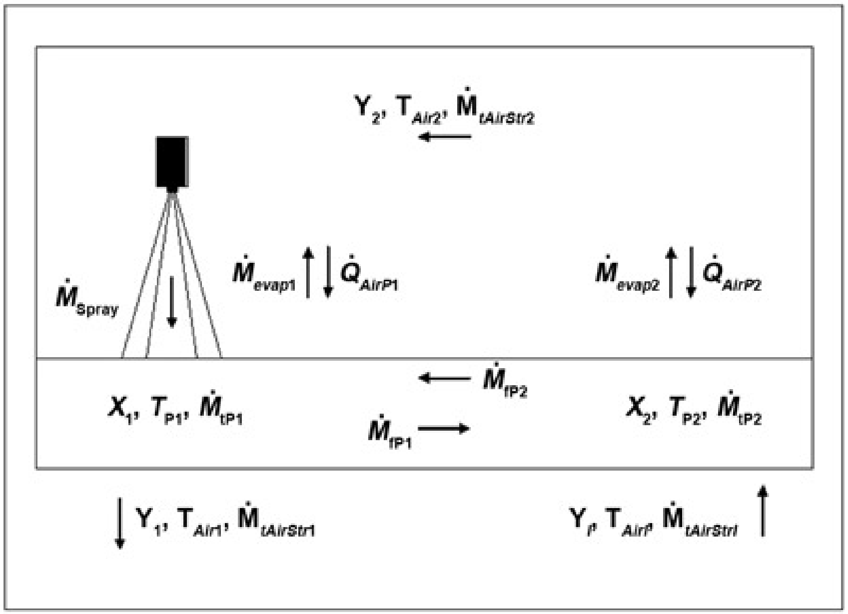

Figure 3. Schematic representation of the heat and mass transfer in the Bohle Lab-Coater (indices: 1 = spray zone, 2 = drying zone, I = air inlet). $\dot{M}_{tPj}$ is the mass of dry tablets (product) in zone j, Xj is the moisture of the tablets in zone j, T_{Pj} is the temperature of the product (tablets) in °C in zone j, $\dot{M}_{fPj}$ is the mass flow of tablets (product) from zone j, $\dot{M}_{Spray}$ is the spray rate, $\dot{Q}_{AirPj}$ is the heat flow from the air to the product (tablets) in zone j, $\dot{M}_{evapj}$ the evaporation rate in zone j, Yj is the air humidity in zone j, T_{Airj} the temperature of the air in zone j and $\dot{M}_{tAirStrj}$ is the mass flow of dry air from zone j.

Balance Equations for the Spray Zone (Zone 1)

The moisture of the tablets in the spraying zone is influenced by different subprocesses. The moisture content of the tablets increases while spraying an aqueous solution or dispersion onto the tablet bed ($\dot{M}_{Spray}$ − spray rate in kg/s). In addition, there is a small increase in the moisture content owing to tablets entering the spray zone with a certain remaining moisture ($\psi_2\ M_{tP2}\ X_2(t)$—herein ψ_2 means the exchange rate of the tablets leaving zone 2 in 1/s, M_{tP2} is the mass of the dry tablets in kilograms (product), and X_2 is the moisture of the tablets in kg/kg in zone 2). The moisture of the tablet decreased owing to the removal of wet tablets from the spraying zone ($\psi_1\ M_{tP1}\ X_1(t)$—herein ψ_1 means the exchange rate of the tablets leaving zone 1 in 1/s, M_{tP1} is the mass of the dry tablets in kilograms (product), and X_1 is the moisture of the tablets in kg/kg in zone 1) and resulting from the evaporation of water from the tablet surface ($\dot{M}_{evap1}$ indicates the evaporation rate in zone 1 in kg/s). The moisture content of the product as a function of time can therefore be described using the following differential equation:

$$M_{tP1}\frac{dX_1(t)}{dt} = \dot{M}_{Spray} - \dot{M}_{evap1} - \psi_1\ M_{tP1}\ X_1(t) + \psi_2\ M_{tP2}\ X_2(t). \quad (1)$$

The air humidity in the spraying zone changes also during the coating process. The air absorbs the evaporated water from the surface of the tablets ($\dot{M}_{evap1}$ indicates the evaporation rate in zone 1), and it changes owing to air entering and leaving this zone ($\dot{M}_{tAirStr2}Y_2(t) - \dot{M}_{tAirStr1}Y_1(t)$—herein $\dot{M}_{tAirStrj}$ is the mass flow of dry air from zone j in kg/s and Y_j is the air humidity in zone j in kg/kg), which makes the following equation valid:

$$M_{tAir1}\frac{dY_1(t)}{dt} = \dot{M}_{evap1} + \dot{M}_{tAirStr2}\ Y_2(t) - \dot{M}_{tAirStr1}Y_1(t). \quad (2)$$

The changes in the product and air temperature in the spraying zone can be calculated from the balance equations of their enthalpies. The following differential equations describe the enthalpy of the product

$$\begin{aligned} M_{tP1}\left\{[c_{pP}(t) + X_1(t)\ c_{pF}]\ \frac{dT_{P1}(t)}{dt} + c_{pF}\ T_{P1}(t)\ \frac{dX_1(t)}{dt}\right\} \\ = \dot{M}_{Spray}\ c_{pF}\ T_{Spray} + \dot{Q}_{AirP1} - \dot{M}_{evap1}\ [\Delta h_V^\circ + c_{pP}(t)T_{P1}(t)] \\ - \psi_1\ M_{tP1}\ [c_{pP}(t) + X_1(t)\ c_{pF}]\ T_{P1}(t) \\ + \psi_2\ M_{tP2}\ [c_{pP}(t) + X_2(t)\ c_{pF}]\ T_{P2}(t) \end{aligned} \quad (3)$$

and the air as a function of time.

$$\begin{aligned} M_{tAir1}\left\{[c_{pAir} + Y_1(t)\ c_{pV}]\ \frac{dT_{Air1}(t)}{dt} + c_{pV}\ T_{Air1}(t)\ \frac{dY_1(t)}{dt}\right\} \\ = \dot{M}_{evap1}\ [\Delta h_V^\circ + c_{pV}\ T_{P1}(t)] \\ + \dot{M}_{tAirStr2}\ \{c_{pAir}\ T_{Air2}(t) + Y_2(t)\ [\Delta h_V^\circ + c_{pV}\ T_{Air2}(t)]\} \\ - \dot{M}_{tAirStr1}\ \{c_{pAir}\ T_{Air1}(t) + Y_1(t)\ [\Delta h_V^\circ + c_{pV}\ T_{Air1}(t)]\} \\ - \dot{Q}_{AirP1}. \end{aligned} \quad (4)$$

Herein $\dot{M}_{tPj}$ is the mass of dry tablets (product), c_{pP} is the specific heat capacity of the product in J/(kg K), X_j is the moisture of the tablets in zone j, c_{pF} is the specific heat capacity of the fluid in J/(kg K), T_{Pj} is the temperature of the product (tablets) in °C in zone j, t is the time, $\dot{M}_{Spray}$ is the spray rate, T_{Spray} is the temperature of the spraying liquid, $\dot{Q}_{AirPj}$ is the heat flow from the air to the product (tablets) in zone j in J/s, $\dot{M}_{evapj}$ is the evaporation rate in zone j, Δh_V° is the specific enthalpy of evaporation at 0°C, ψ_j is the exchange rate of the tablets leaving zone j, $\dot{M}_{tAirj}$ is the mass of dry air in zone j, c_{pAir} is the specific heat capacity of the air in J/(kg K), Y_j is the air humidity in zone j, c_{pV} is the specific heat capacity of the vapor in J/(kg K), T_{Airj} is the temperature of the air in zone j, and $\dot{M}_{tAirStrj}$ is the mass flow of dry air from zone j. The temperature of the film on the surface of the tablet that is necessary for the calculation of the mass transfer from the tablets into the air is approximately the tablet bed temperature.

Balance Equations for the Drying Zone (Zone 2)

As in the spraying zone, the balance equation for the drying zone can be analogously derived. In comparison to the equations of the spraying zone, all terms with the index spray have been left out because they belong to the spraying process that only takes place in the spraying zone. The following equation could therefore be drawn for the change in tablet moisture in zone 2 as a function of time:

$$M_{tP2}\,\frac{dX_2(t)}{dt} = -\dot{M}_{evap2} + \psi_1\,M_{tP1}\,X_1(t) - \psi_2\,M_{tP2}\,X_2(t). \quad (5)$$

For the change of air humidity, the following equation could be set up:

$$M_{tAir2}\,\frac{dY_2(t)}{dt} = \dot{M}_{evap2} + \dot{M}_{tAirStrI}\,Y_I(t) - \dot{M}_{tAirStr2}\,Y_2(t). \quad (6)$$

There are also 2 balance equations for the enthalpy of the tablets

$$\begin{aligned} M_{tP2}\left\{[c_{pP}(t) + X_2(t)\,c_{pF}]\,\frac{dT_{P2}(t)}{dt} + c_{pF}\,T_{P2}(t)\,\frac{dX_2(t)}{dt}\right\} \\ = \dot{Q}_{AirP2} - \dot{M}_{evap2}\,[\Delta \overset{\circ}{h}_V + c_{pP}(t)T_{P2}(t)] + \psi_1\,M_{tP1}\,[c_{pP}(t) \\ + X_1(t)\,c_{pF}]\,T_{P1}(t) - \psi_2\,M_{tP2}\,[c_{pP}(t) + X_2(t)\,c_{pF}]\,T_{P2}(t) \quad (7) \end{aligned}$$

and the air as a function of time

$$\begin{aligned} M_{tAir2}\left\{[c_{pAir} + Y_2(t)\,c_{pV}]\,\frac{dT_{Air2}(t)}{dt} + c_{pV}\,T_{Air2}(t)\,\frac{dY_2(t)}{dt}\right\} \\ = \dot{M}_{evap2}\,[\Delta \overset{\circ}{h}_V + c_{pV}\,T_{P2}(t)] + \dot{M}_{tAirStrI}\,\{c_{pAir}\,T_{AirI}(t) \\ + Y_I(t)\,[\Delta \overset{\circ}{h}_V + c_{pV}\,T_{AirI}(t)]\} - \dot{M}_{tAirStr2}\,\{c_{pAir}\,T_{Air2}(t) \\ + Y_2(t)\,[\Delta \overset{\circ}{h}_V + c_{pV}\,T_{Air2}(t)]\} - \dot{Q}_{AirP2}, \quad (8) \end{aligned}$$

which can be used for the calculation of the product and air temperatures. Herein $\dot{M}_{tPj}$ is the mass of dry tablets (product), X_j is the moisture of the tablets in zone j, t is the time, $\dot{M}_{evapj}$ is the evaporation rate in zone j, ψ_j is the exchange rate of the tablets leaving zone j, $\dot{M}_{tAirj}$ is the mass of dry air in zone j, Y_j is the air humidity in zone j, $\dot{M}_{tAirStrj}$ is the mass flow of dry air from zone j, c_{pP} is the specific heat capacity of the product, c_{pF} is the specific heat capacity of the fluid, T_{Pj} is the temperature of the product (tablets) in zone j, $\dot{Q}_{AirPj}$ is the heat flow from the air to the product (tablets) in zone j, Δh_V° is the specific enthalpy of evaporation at 0°C, c_{pAir} is the specific heat capacity of the air, c_{pD} is the specific heat capacity of the vapor, and T_{Airj} is the temperature of the air in zone j.

Some of the variables in the balance equations are temperature dependent. These variables are the heat capacity c_{pAir} of the air, the heat capacities of the water c_{pF}, the water vapor c_{pV}, and the product c_{pP} (tablets, capsules). Owing to a low temperature influence on the heat capacity, the first 3 parameters are assumed to be constant. There is only one exception: the heat capacity of the tablets is calculated in dependence of temperature, since large differences between both zones will have an influence on the calculations. The equations to calculate the temperature-dependent heat capacity of the tablets were derived from experimental determinations. This variable is also dependent on the composition of the tablets.

Mass and Heat Transfer by Convection

Heat Transfer

Heated air is used to evaporate the dispersing agent in the polymer preparation. After removing the dispersing agent, the film is formed on the surface. As mentioned earlier, the heat transfer from the air to the tablets is done by convection and can be described by the following equation[7]:

$$\dot{Q}_{AirPj} = \alpha\,A_{oj}\,(T_{Air} - T_P), \quad (9)$$

where α is the heat transfer coefficient in W/(m² K), A_{oj} is the surface in m² at which the heat transfer takes place (this is constant during a coating process in contrast to a granulation process), and $T_{Air} - T_P$ is the temperature difference between the air and the boundary layer (tablet surface).

The coefficient of heat transfer α depends on the current velocity of the air, the size of the streaming body characterized by its characteristic length L in mm, and the physical parameters of the fluid (air). It could be calculated from the Nusselt-Number using the following correlation, where λ_{Air} is the heat conductivity in W/(m K):

$$Nu = \frac{\alpha\,L}{\lambda_{Air}} \quad (10)$$

The characteristic length of the body L depends on its shape. For spherical bodies it is as follows[8]:

$$L = \frac{\pi\, d^2}{\pi\, d} = d \tag{11}$$

with d in millimeters as the diameter.

The Nusselt-Number Nu could be calculated from the superposition of the expressions for the laminar and the turbulent flow (the Nusselt-Number for the stagnated medium can be neglected). That means the Nusselt-Number was calculated using the following equations:

$$Nu = \sqrt{Nu_{lam}^2 + Nu_{turb}^2} \tag{12}$$

$$Nu_{lam} = 0.664 Re^{1/2} Pr^{1/3} \tag{13}$$

$$Nu_{turb} = \frac{0.037\; Re^{0.8} Pr}{1 + 2.443\; Re^{-0,1}(Pr^{2/3} - 1)} \tag{14}$$

for the Reynolds-Number Re

$$Re = \frac{w_S\; \rho_{Air}\; L}{\eta_{Air}} \tag{15}$$

and for the Prandtl-Number Pr

$$Pr = \frac{\eta_{Air}\; c_{pAir}}{\lambda_{Air}}\; . \tag{16}$$

In the definition of the Reynolds-Number, w_s is the velocity in the center of the fluid in m/s, and it was calculated from the air flow rate, the gap volume of the particle bulk, and the area of the inlet air duct. ρ_{Air} is the density of the air in kg/m³; L, the characteristic length of a particle; η_{Air}, the dynamic viscosity of the air in kg/(m s); c_{pAir}, the specific heat capacity of the air; and λ_{Air}, the heat conductivity.

The surface at which the heat transfer takes place (A_{oj}) is assumed to be the surface area of all tablets in this zone and can therefore be calculated from the number of tablets in this zone and the surface area of one tablet. The drying behavior of different materials can be described using the parameters limit moisture and critical moisture. The critical moisture indicates the transition from the first to the second section of the drying characteristic, whereas the limit moisture describes the moisture at the end of the second drying section. Both parameters mainly depend on the drying conditions. Usually, they should be determined using a classical kinetic experiment. In the current case it was not possible to determine these values because of experimental limitations. Instead of the experimental determination of these parameters, they had to be calculated by adapting the measured to the calculated temperatures in both zones.

Mass Transfer

Similar to the characteristic numbers from the heat transfer there are also some for the mass transfer. These are the Reynolds-Number Re, the Sherwood-Number Sh, and the Schmidt-Number Sc. The last ones are defined as follows:

$$Sh = \frac{\beta\, L}{\delta} \tag{17}$$

and

$$Sc = \frac{\nu}{\delta}\,. \tag{18}$$

In these equations, β is the mass transfer coefficient in m/s, L is the characteristic length of the particle, δ is the coefficient of diffusion in m²/s, and ν is the kinematic viscosity in m²/s. Owing to similar implementations between heat transfer and mass transfer, and under the assumption that in gas approximately Pr = Sc, the heat-transfer coefficient could be calculated according to Weiss et al[8]:

$$\beta = \frac{\alpha}{c_{pAir}\; \rho_{Air}}\,. \tag{19}$$

Here c_{pAir} is the specific heat capacity in air at a constant pressure, and ρ_{Air} is the density of the air. Using similar implementations, it is possible to calculate the amount of water that changes from the tablet surface into the air. For the special case of evaporation of water in flowing air, the mass transfer can be calculated according to Equation 20. Herein, M_V^- is the molar mass of water vapor and M_A^- is the molar mass of air. A detailed description can be found in the literature.[9]

$$M_{evap} = A_0 \rho_L \frac{M_V^-}{M_A^-}\, \beta\, \frac{1 + \frac{M_A^-}{M_V^-} Y_*}{1 + \frac{M_A^-}{M_V^-} Y_A} \tag{20}$$

The humidity of the air Y_A is equal to the air humidity in this part of the drum, whereas the humidity at the phase interface Y_* can be calculated from the equilibrium partial vapor pressure p_* at the phase interface according to the following equations:

$$Y_* = \frac{\frac{p_*}{10000}}{1 - \frac{p_*}{10000}} \tag{21}$$

$$p_* = exp(23.462 - \frac{3978.205}{233.349 + T_P}) \tag{22}$$

Some of the variables are temperature dependent. These variables are the density ρ_{Air}, the viscosity υ_{Air}, the heat conductivity λ_{Air}, and the heat capacity c_{pAir} of the air. Owing to a low temperature influence, these parameters are assumed to be constant.

Generalization for Inclined Drums

In a horizontal position of the drum, both zones are loaded with the same amount of tablets. However, some commercial coating pans (such as the Bohle Lab-Coater) are designed to be inclined or tilted during the process to help improve tablet convection and mixing dynamics. If the drum is inclined during the process, the tablets move to the lower part of the drum, so that this part contains more than half of the batch size. There is a replacement of tablets between both zones when the drum is rotated. The amount of tablets that leaves one zone must be equal to the amount of tablets that enter the other in a given period of time. Therefore the following equation can be set up:

$$\psi_1\ M_{tP1} = \psi_2\ M_{tP2}. \tag{23}$$

The masses M_{tP1} and M_{tP2} could be calculated from the product of the bulk volume of the tablets in this zone (V_l and V_u) and the bulk density ρ_{bulk}. The derivation to calculate the bulk volumes is given below. From preliminary experiments, it is known that the loading proportions of the drum are the same as described in Figure 4.

The total volume of the particle bulk in the drum $V_u + V_l$ could be derived from the integral of the area A over the length H according to Equation 24. The area A depends on the radius of the drum R and the offset $\Delta(y)$, which is the difference between the center of the drum and the height of the bulk. $\Delta(y)$ depends, owing to geometrical reasons, on the offset at y = 0 $\Delta(0)$, on the inclination angle γ in rad, and on the value of y.

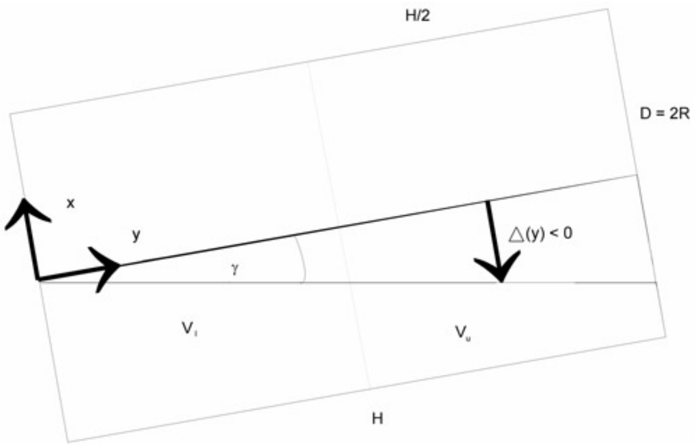

Figure 4. Filling degree in an inclined drum. D diameter of the drum, H length of the drum, γ inclination angle, V_u Volume upper part, V_l Volume lower part, $\Delta(y)$ offset.

$$V = \int_0^H A(R, \Delta(y))\ \ dy \tag{24}$$

and

$$\Delta(y) = \Delta(0) - y\ tan\ \gamma. \tag{25}$$

The area A could be calculated as follows:

$$A = 2\int_{-R}^{\Delta}\sqrt{R^2 - x^2}\ dx. \tag{26}$$

After solving the integral of the area A, the volume can be written with this equation:

$$V = \int_0^H R^2\left(\frac{\Delta(y)}{R}\sqrt{1 - \left(\frac{\Delta(y)}{R}\right)^2} + arcsin\left(\frac{\Delta(y)}{R}\right) + \frac{\pi}{2}\right)dy. \tag{27}$$

The solution of this integral is

$$V = \frac{1}{tan\ \gamma}\left[\frac{1}{3}(R^2 - \Delta^2)^{3/2} - R^2\sqrt{R^2 - \Delta^2} - \Delta\ R^2 arcsin\left(\frac{\Delta}{R}\right)\right]_{\Delta(0)}^{\Delta(0) - H\ tan\ \gamma} \tag{28}$$

Using this equation, the offset at y = 0 $\Delta(0)$ can be calculated from the total bulk volume. With this knowledge, the bulk volume of the tablets in both parts of the drum could be calculated using the inclination angle. Therefore, the bulk volume of the tablets in the lower part is

$$V_l = \frac{1}{tan\ \gamma}\left[\frac{1}{3}(R^2 - \Delta^2)^{3/2} - R^2\sqrt{R^2 - \Delta^2} - \Delta\ R^2 arcsin\left(\frac{\Delta}{R}\right)\right]_{\Delta(0)}^{\Delta(0) - H/2\ tan\ \gamma} \tag{29}$$

and in the upper part

$$V_u = \frac{1}{tan\ \gamma}\left[\frac{1}{3}(R^2 - \Delta^2)^{3/2} - R^2\sqrt{R^2 - \Delta^2} - \Delta\ R^2 arcsin\left(\frac{\Delta}{R}\right)\right]_{\Delta(0) - H/2\ tan\ \gamma}^{\Delta(0) - H\ tan\ \gamma} \tag{30}$$

Thus, based on the bulk volume in each zone and the bulk density, the amount of tablets could be calculated for each zone.

Description of the Transverse Mixing

In the literature, different approaches for the mathematical description of the movement of granular materials in rotated drums can be found.[10,11] Bed behavior diagrams are used for the illustration of the movement. A direct application of these models on the motion of the tablets in the drum of the Bohle Coater is impossible, because those models were developed for drums without mixing devices (such as rotary kilns), or the movement took place only in one direction. In most cases, only the rolling mode is considered. In the current case, the mixing takes place by cascading and by the mixing ribbons that are fitted to the drum wall.

Another approach for the description of the movement of tablets inside a coating drum is based on the discrete element method.[12] In this case, the trajectories of individual particles are calculated by Newton's equation of motion, which considers the contact forces with neighboring particles. This method requires a high level of calculations and computational power and could therefore have limitations for rapid calculation of simulations with higher batch loads and larger tablet numbers.

For the model described in this article the exchange of the tablets between both zones is most important. This exchange is described in the differential equations as exchange rate ψ_j. However, there is a correlation between both exchange rates (see Equation 23).

The movement of the tablets from zone 1 to zone 2 is relatively unhindered, whereas the product flow in the opposite direction is much more difficult because of the pressure caused by the bed of tablets. The derivation of the exchange rate is therefore done for ψ_2. For the calculation of the exchange rate ψ_2 it is necessary to know the filling degree (height of the tablet bulk; *f* in Figure 5). Therefore, the area of the circle segment A_{KA} must be calculated from the batch size $M_{tP1} + M_{tP2}$, the bulk density ρ_{bulk}, and the length of the cylindrical part of the drum H:

$$A_{KA} = \frac{M_{tP1} + M_{tP2}}{\rho_{bulk}\, H}. \tag{31}$$

The area of the circle segment A_{KA} results from the difference between the circle sector A_{KS} and the isosceles triangle A_{DE} with the angle 2ω (red triangle in Figure 5). From this knowledge and from the height of the tablet bulk f the angle ω could be calculated. This is necessary for the determination of the exchange rate as described below.

$$A_{KA} = A_{KS} - A_{DE} \tag{32}$$

$$A_{KA} = \omega R^2 - (R - f)^2 \tan\,\omega \tag{33}$$

$$A_{KA} = R^2(\omega - \sin\,\omega\ \ \cos\,\omega) \tag{34}$$

Two inner and 3 outer mixing ribbons are fitted to the drum wall to allow a good horizontal mixing. According to theoretical considerations, only the volume of tablets between these ribbons or a part of this could be transported into the other zone. Both mixing ribbons (index out and in) are contrary. From the height of the tablet bulk and from the geometrical parameters R, h_{out}, h_{in}, and h_{base}, the circle area of the inner ribbon, which is covered by tablets, A_P could be calculated. Therefore the bulk volume of tablets between the inner ribbon in one zone V_P is the circle area covered by the tablets multiplied by the half-length of the drum $H/2$. The exchange rate ψ_2 could then be calculated from the ratio of V_P to the bulk volume of the tablets in the drum, the pan speed n in rpm, and the constant c_{ψ_2}, which describes the part of the volume V_P that will be exchanged during one rotation:

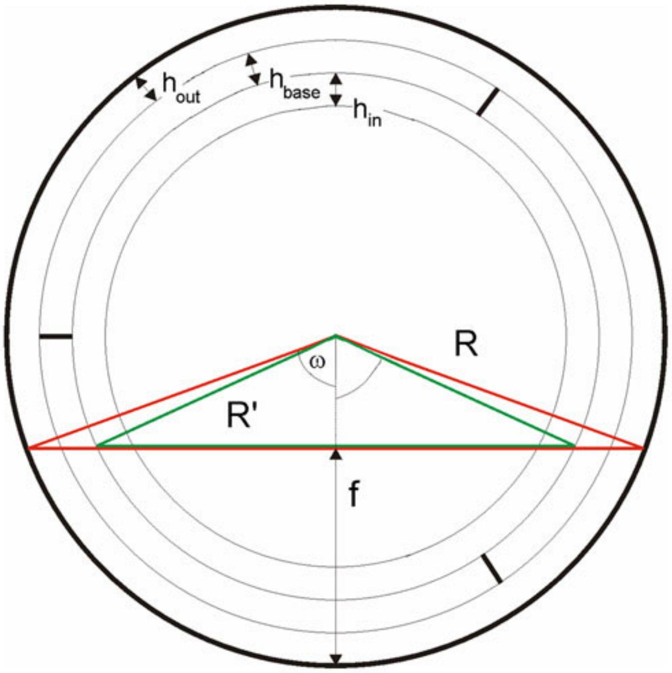

Figure 5. Height of the tablet bulk *f*. *f* height of the tablet bulk, R radius to the outer ribbon, R′ radius to the inner ribbon, h_{out} height outer ribbon, h_{base} height of the base for the inner ribbon, h_{in} height inner ribbon, ω angle.

$$\psi_2 = c_{\psi_2} \frac{V_P\, \rho_{bulk}}{M_{tP1} + M_{tP2}}\, n \tag{35}$$

$$V_P = \frac{A_P H}{2} \tag{36}$$

The constant c_{ψ_2} has to be determined by adaptation of the model by parameter optimization.

Calculation of Further Variables

Besides the variables from the movement and from the heat and mass transfer, there are some other variables that are already mentioned in the balance equations. The calculation of these variables is given below. For the calculation of the mass of dry air M_{tAirj} in kilograms, the drum was assumed to be a cylinder (length H and diameter D). From the cylinder volume, the bulk volume of the tablets V_{bulkj} is subtracted.

$$M_{tAirj} = \left(\frac{\pi}{8}D^2H - V_{bulktj}\right)\rho_{Air} \tag{37}$$

In this case the density of the air is the density at the temperature at time $t = 0$.

The following equations were used to calculate the mass of drying air $M_{tAirStr}$, the inlet air flow V in m³/h, and the density of the air at the inlet air temperature.

$$\dot{M}_{tAirStrI} = V\ \rho_{Air}(T_I) \tag{38}$$

$$\dot{M}_{tAirStrI} = \dot{M}_{tAirStr1} = \dot{M}_{tAirStr2} \tag{39}$$

For the determination of the water content in the inlet air based on the Antoine vapor-pressure correlation (Equation 40), the mean room temperature and humidity before and after the process are used[13,14]:

$$p_S = 10^{10.19625 - \frac{1730.63}{T_{room}+233.426}} \tag{40}$$

$$p_V = \frac{rH_{room}\ p_S}{100\%} \tag{41}$$

$$Y_I = 0.622\frac{p_V}{p_{tot} - p_V} \tag{42}$$

with p_s as saturated vapor pressure in Pa; p_v as partial vapor pressure in Pa; rH_{room} as relative humidity in percentage; and p_{tot} as total pressure in Pa.

CONCLUSION

For the derived model, all relevant parameters could either be calculated or measured, except the constant c_{ψ_2} for the calculation of the exchange rate ψ_2, the critical moisture x_k and the limit moisture x_G. These parameters have to be determined by adaptation of a set of experiments. This method is described in detail in part II of the article. Furthermore, the final model will be applied to existing data in order to check its validity.

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