Mathematical modeling of heat and mass transfer of particles encapsulation in a fluidised bed

Modelowanie matematyczne wymiany ciepła i masy w procesie pokrywania cząstek w złożu fluidalnym

Abstract
The mathematical model, which allows to predict changes of the coverage degree, the moisture content and temperature of particles in process time, was developed. Taking into account changes of the evaporation surface due to an increasing particles coverage degree in the encapsulation process allows to describe the evolution of particles parameters more adequately and to select of process rational parameters.

Keywords: modelling, encapsulation, heat and mass transfer, the degree of coverage, fluidised bed

Streszczenie
Zaproponowano rozbudowany model matematyczny, który umożliwia wyznaczenie zmiany stopnia pokrycia, zawartości wilgoci i temperatury cząstek podczas ich pokrywania w złożu fluidalnym. Na podstawie zmian powierzchni parowania spowodowanych zwiększeniem stopnia pokrycia cząstek model ułatwia bardziej precyzyjny opis zmian ich parametrów oraz odpowiedni dobór parametrów procesowych.

Słowa kluczowe: modelowanie, pokrywanie cząstek, wymiana ciepła i masy, stopień pokrycia, złoże fluidalne
1. **Introduction**

Encapsulation of various particulate materials by shells protects them from the environment, provides a controlled release of the active substance and extends the shelf life of perishable and unstable substances [1].

There are several possible encapsulation methods, e.g. encapsulation by polycondensation and polymerisation on the particles surface, spray drying, spraying, pressing, extrusion, etc. [1].

In this paper, encapsulation of granulated fertilisers into polymeric shells in a fluidised-bed apparatus was carried out. Encapsulation was performed by spraying styrene acrylic polymer dispersion on particles of a fluidised bed. The amount of dispersion was 10–30% by weight of the granules. Drops of dispersion having faced with granules, spread over their surfaces and form a liquid film. Removal of the solvent by drying leads to solidification of film.

The process was carried out in the spouted bed. It provides intensive particle circulation. This way, conditions are created for a multiple passage of each particle through the nozzles irrigation area. It facilitates uniform distribution of the film-forming material over the surface of the treated granules.

The scheme of the laboratory installation for producing of encapsulated granules of mineral fertilisers is presented in Fig. 1. The fluidised bed apparatus has a cylindrical and tapered shape, with 70 mm in lattice diameter. Height of tapered part of the apparatus is 400 mm. Diameter of the top cylindrical part is 210 mm.

![Fig. 1. Scheme of laboratory installation: 1 – fluidised bed apparatus, 2 – electric heater, 3 – voltage controller, 4 – cyclone, 5 – rotameter, 6 – blower, 7 – temperature measurer, 8 – nozzle, 9 – diaphragm compressor, 10 – dosing pump, 11 – tank for dispersion of shell former](image-url)
This size ratio facilitates the organisations of the so-called air-fountain fluidisation mode. When the gas stream rises through a gas distributor plate in a bed of particles, a gas stream gushes along the vertical axis of the apparatus, taking upwards the part of granules. As granules move up, the gas velocity decreases and the granules movement slow down. When the particles reach a certain height, they fall in the peripheral zone, and roll down along apparatus walls to the gas distributor plate. Near the distributor plate, they are taken upwards again by the rising gas stream.

Fluidising agent (air) is heated by an electric heater 2. The temperature control is performed by changing the amperage through the electric heater coil with a voltage controller 3. Atmospheric air is pumped to electric heater by blower 6. Rotameter 5 serves to control the air flow. Intensive motion of particles in the apparatus 1 in a spouted bed mode may cause attrition. Cyclone 4 serves to clean the air flowing out of the apparatus from dust fraction of the treated product.

A fine polymer dispersion spraying is provided by pneumatic nozzle 8. The polymer emulsion is dosed into the nozzle by peristaltic pump 11 from the tank 10. Compressed air is supplied to the nozzle by a membrane compressor 9. The temperature measurer 7 allows to control the temperature of the granules bed in the apparatus. A thermocouple is used as a temperature sensor.

2. Mathematical model

Traditionally, in the simulation of drying particulate materials, the evaporating surface is assumed to be the surface area of the particles. The surface area of evaporation $F_{\text{evap}}$ changes constantly in time during the encapsulation of particles (batch process).

$$F_{\text{evap}} = \pi \cdot d_{\text{av}}^2 \cdot N \cdot x_{\text{av}}$$  (1)

where:

- $d_{\text{av}}$ – average diameter of particles,
- $N$ – the number of particles in the bed.

The degree of particle coating is defined as the part of the total surface of the particles coated with a protective shell in batch mode. It can be calculated by the formula [2]:

$$x_{\text{av}} = \frac{k_4 \cdot \left[ z_2 - z_1 - z_2 \cdot \exp(z_1 \cdot \tau) + z_1 \cdot \exp(z_2 \cdot \tau) \right]}{z_1 \cdot z_2 \cdot (z_2 - z_1)}$$  (2)

where:

- $k_1 = - k_2$; $k_2 = k_3 + k_4$; $k_3 = k_2 \cdot k_4$; $k_4 = k_3 \cdot k_2$; $z_1, z_2$ – the roots of the characteristic equation:

$$z_{1,2} = 0.5 \cdot \left[ k_1 - k_2 \pm \sqrt{(k_2 - k_1)^2 + 4 \cdot (k_1 \cdot k_2 + k_3)} \right]$$  (3)
where:

- $k_b$ – the relative flows of particles through the “bed” zone;
- $k_t$ – the relative flows of particles through the “torch” zone;
- $k_\lambda$ – a constant growth rate of the degree of coverage:

$$k_\lambda = \frac{n_d \cdot K_s \cdot g_s^2}{4 \cdot N_t \cdot d_{av}^2} \quad (4)$$

where:

- $d_d$ – drops diameter,
- $n_d$ – number of drops, produced by nozzle per unit time,
- $N_t$ – number of granules in the torch nozzle area,
- $K_s$ – spreading coefficient.

$$n_d = \frac{6 \cdot G_{disp}}{\pi \cdot \rho_{disp} \cdot d_d} \quad (5)$$

where:

- $G_{disp}$ – mass flow of dispersion,
- $\rho_{disp}$ – dispersion density.

$$k_b = \frac{n_t}{N_b} = \frac{1}{\tau_c}, \quad k_t = \frac{n_t}{N_t} \quad (6)$$

where:

- $n_t$ – amount of particles, circulating through the irrigation zone per unit time;
- $N_b, N_t$ – amount of particles in zones “bed” and “torch”, respectively;
- $\tau_c$ – particles circulation period.

$$N_t = \frac{3 \cdot M_t}{\pi \cdot \rho_p \cdot d_{av}^3} \quad (7)$$

where:

- $M_t$ – the mass of particles in the nozzle area,
- $\rho_p$ – particle density.

Period of circulation is calculated as follows [3]:

$$\tau_c = \frac{6.58 \cdot H \cdot (1 - \varepsilon)}{c_1 \cdot V_s \cdot (1 - \varepsilon_t)} \cdot \sqrt{\frac{\rho_p \cdot d_p}{k_f \cdot \rho_{gas} \cdot \left( H + \frac{1.1 \cdot V_0 \cdot r_0}{c_1 \cdot V_s} \right)}} \quad (8)$$

The mass flow of the particles through the torch $G_t$ of nozzle and the mass of particles in the torch area $M_t$ are determined by [3]:

$$G_t = \frac{0.1 \cdot \pi \cdot V_0^2 \cdot r_0^2 \cdot (1 - \varepsilon_t)}{V_s} \cdot \sqrt{\frac{k_f \cdot \rho_{gas} \cdot \rho_p \cdot d_p}{H + \frac{1.1 \cdot V_0 \cdot r_0}{c_1 \cdot V_s}}} \quad (9)$$
\[ M_i = \frac{0.33 \cdot \pi \cdot r_p \cdot V_o^2 \cdot r_o^2 \cdot (1 - \varepsilon_t)}{c_1 \cdot V_a^3} \left[ \frac{1}{2} - \frac{2 \cdot g \cdot d_p \cdot (\rho_p - \rho_{gas})}{2 \cdot g \cdot d_p \cdot (\rho_p - \rho_{gas})} \cdot \frac{L_i}{H} \right] \]  

(10)

\[ L_i = \frac{V_0 \cdot r_0}{0.366 \cdot V_a \cdot c_1} \]  

(11)

\[ c_1 = 0.46 \left( \frac{g \cdot d_p^3}{v_{gas}^2} \right)^{0.1} \cdot W^{0.32} \]  

(12)

where:

- \( \rho_{gas}, \rho_p \) – densities of gas and solid particles, respectively;
- \( \nu_{gas} \) – kinematic coefficient of viscosity of gas;
- \( d_p \) – particles diameter;
- \( H \) – operating height of fluidised bed;
- \( \varepsilon \) – bed porosity;
- \( W \) – fluidisation velocity;
- \( V_s \) – lift velocity;
- \( k_f \) – coefficient of aerodynamic resistance;
- \( V_0, r_0 \) – initial velocity and radius of gas jet;
- \( \varepsilon_t \) – porosity of “gas-solids” area of nozzle torch;
- \( g \) – acceleration of gravity;
- \( c_1 \) – empirical coefficient.

The mass of particles increases when dispersion droplets contact with the particles’ surface. At the same time, due to evaporation of the solvent (water), the mass decreases. Since water evaporates from a thin film, we accept the assumption that the process of mass transfer is limited by external diffusion. The ratio of total moisture weight to the total weight of dry material was taken for quantitative characterisation of the particles’ moisture content \( U \):

\[ U = \frac{m_p \cdot U_p + m_{polym} \cdot U_f}{m_p + m_{polym}} \]  

(13)

where:

- \( m_p \) – mass of original granule;
- \( U_p \) – granule moisture content;
- \( m_{polym} \) – weight of the polymer in the polymer film on the granule;
- \( U_f \) – film moisture content.

The initial moisture content of the film \( U_{f,0} \) is calculated by:

\[ U_{f,0} = \frac{1 - B_{polym}}{B_{polym}} \]  

(14)

where:

- \( B_{polym} \) – the mass fraction of the polymer in the emulsion.
The denominator of the right side of formula (13) is a mass of dry material in the bed of encapsulated particles at the moment of time $\tau$:

$$m_{dry} = m_p + G_{disp} \cdot B_{polym} \cdot \tau \quad (15)$$

Change of the moisture content per unit of time:

$$\frac{d(U \cdot m_{dry})}{d\tau} = \frac{d}{d\tau} \left( U \cdot \left( m_p + G_{disp} \cdot B_{polym} \cdot \tau \right) \right) \quad (16)$$

where:

$G_{disp}$ – dispersion mass flow,

$\tau$ – time.

Differentiation of equation (16) gives (17):

$$\frac{d(U \cdot m_{dry})}{d\tau} = \left( m_p + G_{disp} \cdot B_{polym} \cdot \tau \right) \frac{dU}{d\tau} + U \cdot G_{disp} \cdot B_{polym} \quad (17)$$

The flow of the evaporated moisture can be calculated by the equation of mass transfer. At the same time, the amount of moisture increases due to inflow of the emulsion.

$$\frac{d(U \cdot m_{dry})}{d\tau} = -\beta_p \cdot \left( P_{surf} - P_{gas} \right) \cdot F_{evap} + G_{disp} \cdot \left( 1 - B_{polym} \right) \quad (18)$$

From equations (17) and (18), we can find the rate of moisture content change:

$$\frac{dU}{d\tau} = \frac{-\beta_p \cdot \left( P_{surf} - P_{gas} \right) \cdot F_{evap} + G_{disp} \cdot \left( 1 - B_{polym} \right) - U \cdot G_{disp} \cdot B_{polym}}{m_p + G_{disp} \cdot B_{polym} \cdot \tau} \quad (19)$$

where:

$\beta_p$ – mass transfer coefficient,

$P_{surf}$ – partial pressure of water vapour over film surface,

$P_{gas}$ – partial pressure of water vapour in the drying agent,

$F_{evap}$ – evaporation surface.

The pressure of water vapour over the film surface depends on the material temperature; therefore, an equation of the thermal balance in differential form is included in the mathematical model.

$$\frac{d}{d\tau} \left( \left( m_p + G_{disp} \cdot B_{polym} \cdot \tau \right) \cdot c_{av} \cdot t \right) = \alpha \left( t_{gas} - t \right) \cdot F_{n.tr.} - \beta_p \left( P_{surf} - P_{gas} \right) \cdot F_{evap} \cdot r \quad (20)$$
where:

- $c_{av}$ – average heat capacity of the particles,
- $F_{h.tr}$ – heat transfer surface,
- $t$ – particles temperature,
- $t_{gas}$ – gas temperature,
- $r^*$ – water vaporisation heat,
- $\alpha$ – heat transfer coefficient.

The rate of temperature change is defined as follows:

$$\frac{dt}{d\tau} = \frac{\alpha(t_{gas} - t) \cdot F_{h.tr} \cdot \beta_p \left( P_{surf} - P_{gas} \right) \cdot F_{evap} \cdot r^* - G_{disp} \cdot B_{poly} \cdot t \cdot c_{av}}{(m_p + G_{disp} \cdot B_{poly} \cdot \tau) \cdot c_{av}}$$

(21)

The system of equations (19) and (21), allows to predict the change of moisture content and temperature of the particles in time of encapsulation process. The evaporation surface of particles depends on the degree of coverage (1) equations (19) and (21) and it must be solved together with the equation (2).

3. Results and discussion

The system of equations (1–21) was solved numerically by means of the Mathcad software. Figures 2a, b show the dependence of the degree of particle coating, the moisture content of film formed, temperature, and the overall moisture content per process time.

![Fig. 2. Particles parameters per process time: a – degree of particle coating $x_{av}$ and moisture content of film $U_f$ per process time $\tau$. b – temperature $t$, and the overall moisture content $U$ per process time $\tau$.](image)

The results of calculations show that at the initial stage of the coating formation, an increasing of temperature and moisture content of particles is observed. It is due to a lack of evaporation surface area. Furthermore, when the degree of coverage of the particles reaches 100%, the moisture content decreases to the initial humidity of the material.
The mathematical model shows the most important features of the process and it can be used for calculation of the fluidised bed apparatus.

References

[1] Ovchinnikov L.N., Lipin A.G., *Encapsulation of fertilizer in fluidized bed: a monograph*, ISUCT, Ivanovo 2011 (in Russian).
[2] Lipin A.G., Ovchinnikov L.N., Fedosov S.V., *Methods of evaluating the quality of granular materials encapsulation in a fluidized bed*, Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol., Vol. 43(1), 2000, 73–75 (in Russian).
[3] Buevich Yu. A., Minaev G.A., *Jet fluidization*, Khimiya, Moscow 1984 (in Russian).