SOLVING THE EQUATION OF MASS TRANSFER IN A STATIONARY BED OF GRANULAR MATERIAL

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A general procedure is proposed for the exact integration of a system of quasilinear differential equations often encountered in problems concerning the convective mass transfer in a bed of granular material with reaction at the surface and in the volume of particles.

Various problems concerning the convective mass transfer in a stationary bed of homogeneous granular material can often be reduced [1-4] to solving the following dimensionless system of differential equations:

$$\frac{\partial\psi}{\partial\eta} = \varkappa F(\psi), \quad \frac{\partial\varkappa}{\partial\xi} = -\varkappa F(\psi). \tag{1}$$

The specific kind of function $F(\psi)$ is determined by the mode of reactions which occur at the surface and in the volume of particles making up the bed [1-5].

We will outline here a general procedure for the exact integration of system (1). Individual problems were earlier solved either as special cases [1] or by numerical methods [2]. The reaction equations (1) apply only to the inside of the reaction zone (Fig. 1), which at a given instant of time is defined by the inequality

$$\xi_*(\eta) > \xi > \xi^*(\eta). \tag{2}$$

The boundaries of the reaction zone† ξ_* and ξ^* are not known a priori and will be determined in the course of the solution. When $\xi > \xi_*(\eta)$, the material has not yet entered into a reaction with the gas and, consequently, $\varkappa = \psi = 0$. On the other hand, the zone of material which has reacted already ($\varkappa = \psi = 1$) is defined by the inequality $\xi < \xi^*(\eta)$.

At a fixed depth ξ the reaction begins at time $\eta = \eta_*(\xi)$, where function $\eta_*(\xi)$ is the inverse of function $\xi_*(\eta)$. Therefore, the initial condition for system (1) can be stated as

$$\psi|_{\eta=\eta_*(\xi)} = \varkappa|_{\eta=\eta_*(\xi)} = 0. \tag{3}$$

We note that $\eta_*(0) = 0$, inasmuch as the reaction at the bed surface begins at $\eta = 0$.

Formulating the boundary conditions is somewhat more difficult. When $\eta < \eta_*(0)$, where function $\eta^*(\xi)$ is the inverse of function $\xi^*(\eta)$, the material at the surface has not yet reacted completely and, therefore, we have a single boundary condition:

$$\varkappa|_{\xi=0} = 1. \tag{4}$$

As a consequence of this condition, from Eq. (1) for $\xi = 0$ follows directly an equation which characterizes the reaction trend in particles at the bed surface:

$$\eta = h(\psi_0) \quad (\psi_0 = \psi|_{\xi=0}), \tag{5}$$

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† For convenience, time and distance will be represented by their dimensionless analogs η and ξ, respectively.

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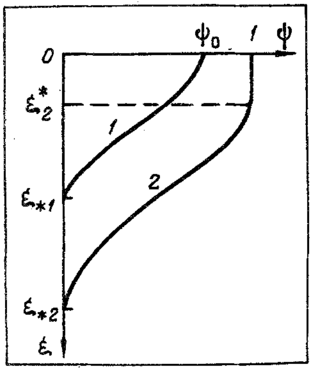

Fig. 1. Distribution of the material conversion factor across the bed thickness at various instants of time: $\eta_1 < \eta^*(0)$, $\eta_2 > \eta_*(0)$.

with

$$h(\psi) = \int_0^{\psi} \frac{d\psi}{F(\psi)}. \tag{6}$$

Function $h(\psi)$ must exist for sufficiently small positive values of ψ. Otherwise, relation (5) would be physically meaningless and the reaction in the particles could not begin. At small values of ψ, therefore, function $F(\psi)$ must behave like ψ^{α}, where α is a real number smaller than unity.

The reaction at the bed surface will be completed at the instant of time

$$\eta^*(0) = h(1). \tag{7}$$

In the physical sense, function $F(\psi)$ is positive and becomes zero when $\psi \to 1$. Therefore, near unity $F(\psi)$ must decrease like $(1-\psi)^{\beta}$ $(\beta > 0)$. Consequently, at $\psi = 1$ integral (6) is an improper one and can exist only on the interval $0 < \beta < 1$. In this case the reaction time at the bed surface $\eta = \eta^*(0)$ is finite (see Eq. (7)). When $\eta > \eta^*(0)$, the reaction zone separates from the geometric surface and the following two boundary conditions apply as a result:

$$\psi|_{\xi=\xi^*(\eta)} = \varkappa|_{\xi=\xi^*(\eta)} = 1. \tag{8}$$

When $\beta \geq 1$, on the other hand, then integral (6) becomes divergent at $\psi = 1$ and the reaction will continue for an infinitely long time $(\eta^*(0) = \infty)$. Moreover, the boundary condition (4) remains valid and toward the end of the reaction is definable only as an approximation within any necessary accuracy.

We note that the emergence of two boundary conditions (8) instead of one (4) at $\eta > \eta^*(0)$ does not make the problem indeterminate because the equation of boundary $\xi = \xi^*(\eta)$ is not known. A similar situation is found in the case of the initial conditions (3).

We will now proceed to the direct integration of system (1) under the constraints (3), (4), and (8). This we begin by rewriting the first of Eqs. (1) as

$$\frac{\partial h}{\partial \eta} = \varkappa \tag{9}$$

and then differentiating it partially with respect to ξ. Then, after some transformations and taking Eqs. (1) into consideration, we obtain

$$\frac{\partial}{\partial \eta}\left(\frac{1}{F(\psi)} \cdot \frac{\partial \psi}{\partial \xi} + \psi\right) = 0. \tag{10}$$

This, together with the initial condition (3), yields

$$\frac{1}{F(\psi)} \cdot \frac{\partial \psi}{\partial \xi} + \psi = \frac{1}{F(\psi)} \cdot \frac{\partial \psi}{\partial \xi}\bigg|_{\eta=\eta_*(\xi)}. \tag{11}$$

Next we differentiate the first initial condition (3) with respect to ξ. This yields

$$\frac{\partial \psi}{\partial \xi}\bigg|_{\eta=\eta_*(\xi)} + \frac{\partial \psi}{\partial \eta}\bigg|_{\eta=\eta_*(\xi)} \frac{d\eta_*}{d\xi} = 0. \tag{12}$$

When $F(0) \neq 0$, it follows directly from relation (12) that

$$\frac{1}{F(\psi)} \cdot \frac{\partial \psi}{\partial \xi}\bigg|_{\eta=\eta_*(\xi)} = -\frac{1}{F(\psi)} \cdot \frac{\partial \psi}{\partial \eta}\bigg|_{\eta=\eta_*(\xi)} \frac{d\eta_*}{d\xi}. \tag{13}$$

As a consequence of the first of Eqs. (1), we have then

$$\frac{1}{F(\psi)} \cdot \frac{\partial \psi}{\partial \xi}\bigg|_{\eta=\eta_*(\xi)} = -\varkappa\bigg|_{\eta=\eta_*(\xi)} \frac{d\eta_*}{d\xi}. \tag{14}$$

Since the lower boundary of the reaction zone shifts at a rate $d\xi_*/d\eta$ which cannot be equal to zero and, therefore, $d\eta^*/d\xi < \infty$ and relation (14), according to the second of initial conditions (3) becomes

$$\frac{1}{F(\psi)} \cdot \frac{\partial\psi}{\partial\xi}\bigg|_{\eta=\eta_*(\xi)} = 0. \tag{15}$$

From the continuity standpoint, this relation is valid also when $F(0) = 0$. Thus, satisfying the initial conditions (3) ensures that the ordinary differential equation

$$\frac{\partial\psi}{\partial\xi} + \psi F(\psi) = 0 \tag{16}$$

will apply to the inside of the reaction zone. Before directly integrating Eq. (16), we let

$$\frac{\partial}{\partial\xi}\ln\frac{\varkappa}{\psi} = 0, \tag{17}$$

which follows directly from (16) and (1). From (17) we have

$$\begin{aligned} \frac{\varkappa}{\psi} &= \frac{\varkappa}{\psi}\bigg|_{\xi=0}, \quad \eta < \eta^*(0), \\ \frac{\varkappa}{\psi} &= \frac{\varkappa}{\psi}\bigg|_{\xi=\xi^*(\eta)}, \quad \eta > \eta^*(0). \end{aligned} \tag{18}$$

From this expression, and in view of the boundary conditions (4), (8), we conclude that

$$\varkappa = \frac{\psi}{\psi_0}, \quad 0 < \eta \leqslant \eta^*(0) \tag{19}$$

applies as long as the reaction at the bed surface is not completed.

On the other hand, after the reaction zone has separated from the bed surface,

$$\varkappa = \psi, \quad \eta \geqslant \eta^*(0). \tag{20}$$

The solution to Eq. (16) and the reaction trend in the bed volume depend mostly on the values of $F(0)$ and of $dF/d\psi|_{\psi=1}$. The character of these quantities can be established by the values of the earlier introduced exponents α and β. Several quantitatively different situations are possible here.

1. Exponent $\beta \geq 1$ and, therefore

$$\frac{dF}{d\psi}\bigg|_{\psi=1} = \begin{cases} 0 & \beta > 1, \\ \text{const} & \beta = 1. \end{cases} \tag{21}$$

Then the instant of time $\eta^*(0)$ (7) moves to infinity, the reaction at the bed surface continues infinitely long, and the upper boundary of the reaction zone $\xi^*(\eta)$ passes through the bed surface. How the material conversion factor varies across the bed thickness is determined, according to Eq. (16), from

$$g(\psi_0, \psi) = \xi, \tag{22}$$

where

$$g(\psi_0, \psi) = \int\limits_{\psi}^{\psi_0} \frac{d\psi}{\psi F(\psi)}, \tag{23}$$

and the conversion factor at the bed surface is determined from relation (5).

1a. Along with inequality $\beta \geq 1$, inequality $0 \leq \alpha < 1$ is also valid. This means that

$$F(0) = \begin{cases} 0 & 0 < \alpha < 1, \\ \text{const} & \alpha = 0. \end{cases} \tag{24}$$

The integral in (23) is here infinite for $\psi = 0$ and, consequently, the reaction zone covers the entire bed ($\xi^*(\eta) = \infty$). Such a situation can occur when the reaction inside an individual particle is intrakinetic (at a variable size of the reaction surface) with autocatalysis ($0 < \alpha < 1$) or without it ($\alpha = 0$). For such trends of the reaction, function $F(\psi)$ can be represented as

$$F(\psi) = \psi^{\alpha}(1-\psi)^{\beta}, \tag{25}$$

where exponent α characterizes the progress of autocatalysis and β characterizes the reduction of the reaction surface per unit particle volume during the reaction. We note that functions $F(\psi)$ of type (25) are often used in equations of formal kinetics [5] where, however, the exponents α and β can be treated in a different manner.

Another example of this kind of mass transfer is the drying of moist granular material in such a bed, where the drying rate of individual particles can be established by the Filonenko method for $m > 1$ [6].

In this case

$$F(\psi) = \frac{(1-\psi)^m}{A + B(1-\psi)^m}, \quad m \equiv \beta > 1 \tag{26}$$

and

$$\varkappa = \frac{t_G - t_M}{t_{Go} - t_M}. \tag{27}$$

The variation of temperature t_M across the bed thickness is disregarded here, which usually does not result in large errors [2].

1b. Inequalities $\beta \geq 1$ and $\alpha < 0$ are satisfied simultaneously. Then, along with (21), we have

$$F(0) = \infty. \tag{28}$$

These limitations predetermine the boundedness of integral (23) at $\psi = 0$ and thus the presence of a lower boundary of the reaction zone:

$$\xi_*(\eta) = g(\psi_0, 0). \tag{29}$$

The rate at which this lower boundary shifts is found by differentiating Eq. (29) with respect to η, with (4) taken into account:

$$\frac{d\xi_*}{d\eta} = \frac{1}{\psi_0}. \tag{30}$$

As η increases in the course of the reaction, the rate decreases monotonically from infinite at $\eta = 0$ and, as in this case, approaches unity asymptotically at $\eta \to \infty$.

We note that, at small values of η, the material conversion factor ψ_0 at the surface is proportional to $\eta^{1/(1-\alpha)}$ accurately down to terms of the highest-order smallness, as follows from Eq. (5). For this reason and with the same degree of accuracy at small values of η, we have

$$\frac{d\xi_*}{d\eta} \sim \eta^{-\frac{1}{1-\alpha}}. \tag{31}$$

This case ($\beta \geq 1$, $\alpha < 0$) is of no practical use and only of purely theoretical interest.

2. Exponent $0 < \beta < 1$ and, therefore

$$\left.\frac{dF}{d\psi}\right|_{\psi=1} = -\infty. \tag{32}$$

In this case the reaction at the bed surface continues for a finite length of time ($\eta_*(0) < \infty$) and, after completion, the reaction zone separates. Moreover, the boundary condition (4) and thus also solution (22) are valid on the interval $0 < \eta < \eta^*(0)$. On the other hand, the boundary conditions (8) apply at $\eta > \eta^*(0)$. Therefore, the result of integrating Eq. (16) will be written here as

$$g(1, \psi) = \xi - \xi^*(\eta). \tag{33}$$

In order to determine the rate at which the upper boundary shifts, we differentiate Eq. (33) partially with respect to η. Then, considering (20), (23), and the first of Eqs. (1), we have

$$\frac{d\xi^*}{d\eta} = 1, \tag{34}$$

from where we obtain the following expression for the upper boundary of the reaction zone, by virtue of $\xi^*|_{\eta=\eta^*(0)} = 0$,

$$\xi^* = \eta - \eta^*(0) \quad (\eta > \eta^*(0)). \tag{35}$$

2a. Both inequalities $0 < \beta < 1$ and $0 \le \alpha < 1$ are satisfied. Moreover, (24) applies and the lower boundary of the reaction zone $\xi_*(\eta)$ moves to infinity. Relation (22) for $\eta < \eta^*(0)$ and relation (33) for $\eta > \eta^*(0)$ define the reaction trend throughout the entire bed half-space.

This case corresponds to a reaction for which function $F(\psi)$ in the equations of formal kinetics is determined according to formula (25) when $0 < \beta < 1$ and $0 \le \alpha < 1$.

2b. Inequalities $0 < \beta < 1$ and $\alpha < 0$ are satisfied simultaneously. Moreover, function $F(\psi)$ satisfies relations (28) and (32), and the width of the reaction zone within the bed of particles is always finite. Relation (22) describes the reaction trend till the instant $\eta^*(0)$, when the upper boundary of the reaction zone separates from the bed surface, and it is valid only for $0 < \xi < \xi_*(\eta)$. Within this time interval, the lower boundary $\xi_*(\eta)$ is determined according to formula (29) and it shifts deeper into the bed at a variable rate $1/\psi_0$ (30).

When $\eta > \eta^*(0)$, the reaction trend follows Eq. (33). The upper boundary $\xi^*(\eta)$ is defined according to (35) and the lower boundary, by virtue of (33) and (35), is defined as

$$\xi_*(\eta) = g(1, 0) + \eta - \eta^*(0). \tag{36}$$

Thus, when $\eta > \eta^*(0)$, the boundaries ξ^* and ξ_* shift at the same unit rates, while the dimensionless thickness of the reaction zone $\xi_* - \xi^*$ and the dimensionless time $\eta^* - \eta_*$ are equal to the quadrature of $g(1, 0)$ (see (23)).

The material conversion factor ψ and thus also the quantity $\varkappa$ equal to it are functions of the difference $\xi - \eta$ of two independent variables in the problem. At $\eta > \eta^*(0)$, therefore, the mass-transfer process acquires the characteristics of a traveling wave.

We note that, because $\psi_0|_{\eta=\eta^*(0)} = 1$, the lower boundary shifts at a rate $d\xi_*/d\eta$ which is continuous at the instant $\eta = \eta^*(0)$.

Characteristic of this case is the reaction of particles within the inner diffusion region. Since the resistance to external diffusion is low here at $\psi > 0$, function $F(\psi)$ can be represented as [3]

$$F(\psi) = \frac{(1-\psi)^{1/3}}{1-(1-\psi)^{1/3}}. \tag{37}$$

A simple analysis of relation (37) shows that here $\alpha = -1$ and $\beta = 1/3$.

In summary, we note that the general solution to system (1) reveals, for functions $F(\psi)$ [7] physically meaningful in specific cases, not only the form of functions $\psi(\xi, \eta)$ and $\varkappa(\xi, \eta)$ but also how the material conversion front moves in a bed of particles at any value of ψ within the interval (0, 1). This makes it possible to almost always locate the boundaries of the reaction zone, even when they theoretically do not exist ($\beta \ge 1$, $0 \le \alpha < 1$). For this purpose, it is sufficient in the derived solution to let ψ be close to unity or to zero within any necessary accuracy. The thus defined approximate boundaries will have the properties described in case 2b, within the same accuracy.

The derived solutions extend automatically to the case of a piecewise continuous function $F(\psi)$. In this case, inside the reaction zone there appear additional movable boundaries which correspond to the respective discontinuities of function $F(\psi)$. Such a situation can prevail, for instance, in a bed of drying moist particles when $0 < \psi < \psi_{cr}$ during the first stage of mass transfer (ψ_{cr} denoting the dehydration factor which corresponds to the first critical moisture content) the drying rate is independent of the moisture content and thus $F(\psi) \equiv 1$. If $0 < \psi_0 < \psi_{cr}$, then, according to formulas (5), (19), and (22), the trend of the drying process is described by the equations

$$\psi = \eta \exp(-\xi) \text{ and } \varkappa = \exp(-\xi). \tag{38}$$

On the other hand, if $\psi_{cr} < \psi_0 < 1$ and, which is equivalent, $\eta > \psi_{cr}$, then the mass transfer at the bed surface follows the relation

$$\eta = \psi_{cr} + \int_{\psi_{cr}}^{\psi_0} \frac{d\psi}{F(\psi)} . \tag{39}$$

The dehydration distribution within the zone immediately adjacent to the bed surface, where $\psi_{cr} < \psi < \psi_0$, follows Eq. (22). The equation of the boundary of this zone (horizontal line $\psi = \psi_{cr}$) is, accordingly,

$$g(\psi_0, \psi_{cr}) = \xi_{cr} \tag{40}$$

At $\xi > \xi_{cr}$, the dehydration factor is smaller than critical and, therefore, Eq. (22) becomes here

$$\xi = \xi_{cr} + \ln \frac{\psi_{cr}}{\psi} \tag{41}$$

We note that, since $F(\psi) = 1$ for small values of ψ, exponent α is equal to zero and, consequently, the boundary of the drying zone (in a semiinfinite bed) moves to infinity.

Thus, it follows from the preceding analysis that solutions to specific mass-transfer problems reduce to determining the quadratures of $g(\psi_0, \psi)$ and $h(\psi_0)$. This operation is performed for any physically meaningful form of function $F(\psi)$.

NOTATION

ψ	is the material conversion factor;
$\varkappa$	is the dimensionless analog of the motive force in the mass-transfer reaction;
η	is the dimensionless time;
ξ	is the dimensionless distance from the bed surface;
$F(\psi)$	is the dimensionless analog of mass transferability in bed particles;
t_{Go}, t_G	are the gas temperature at the bed entrance and inside the bed, respectively;
t_M	is the temperature of evaporation surface of particles in the drying process.

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