Abstract

Abstract of the dissertation of Mikhail Andreevich Babkin on the topic: "Development of a Mathematical Model and Digital Twin of Grinding Processes in a Planetary Mill."

Relevance of the research topic. Grinding processes are essential in industries such as nanomaterials, pharmaceuticals, ceramics, pigments, catalysts, and battery production, where high material quality and uniformity are critical. Planetary mills, known for their high energy efficiency and versatility in ultrafine grinding, present modeling challenges due to their multiphase nature and nonlinear breakage kinetics.

Common modeling approaches—such as the method of moments, discrete element method (DEM), and population balance models (PBM)—have limitations. DEM is computationally intensive, while PBM depends on empirical closure relations tailored to specific materials, reducing general applicability.

To overcome these issues, this study introduces a novel approach based on heterogeneous media mechanics and the variational principle of minimum entropy production. This enables prediction of the particle size resistant to breakage using physical parameters and grinding conditions, providing a physically grounded alternative to empirical methods.

Additionally, the development of a digital twin and VR-based training simulator enhances the practical use of the model for process optimization and education, offering real-time visualization and interactive learning for engineers and students.

The aim of the study is to develop of a mathematical model of the grinding process that reflects the complex set of physicochemical phenomena occurring in a planetary mill; development of software and a digital twin for process optimization and training purposes.

To achieve the set goal, it is necessary to solve the following tasks:

1. Conduct experimental studies of the grinding process in a planetary mill to obtain data on particle size changes and their radial distribution.

2. Based on the integration of heterogeneous media mechanics and the thermodynamics of irreversible processes, determine the structure of driving forces and breakage fluxes.

3. By applying methods from the thermodynamics of irreversible processes (the principle of minimum entropy production), establish a relationship for the diameter of particles resistant to breakage.

4. Using Onsager's relations, derive the structure of the breakage flux and determine the functional dependence for the breakage rate constants.

5. Develop a mathematical model of the kinetics of the breakage process, taking into account experimental data and the derived relationships.

6. Develop a numerical method for solving the integro-differential equation describing the

particle size (volume) distribution density.

7. Develop software for simulating the breakage process.

8. Create a digital twin of the mill capable not only of simulating the grinding process but also serving as a training tool for operators.

Scientific novelty. In the process of completing the dissertation, new scientific results were obtained for the first time:

The structures of the thermodynamic flux and driving force of grinding were obtained, distinguished by the application of a thermodynamic approach.

A method for determining the functional dependence of particle diameter was proposed, characterized by the use of the variational principle of minimum entropy production as a criterion of thermodynamic stability in heterogeneous systems, which makes it possible to determine the diameter of particles resistant to breakage as a function of process parameters.

A functional dependence of the "breakage constant" was found, distinguished by the use of a thermodynamic approach, which allows one to move away from empirical relationships.

An original finite difference scheme was developed for solving the integro-differential population balance equation, taking into account the phenomenon of particle breakage. It is distinguished by the application of the method of fractional steps, enabling a high degree of approximation of the process.

A digital twin of the planetary mill was developed, featuring an integrated mathematical model of grinding kinetics, which provides the ability to train users and conduct computational experiments in virtual reality.

The theoretical and pratical significance. Based on experimental studies of aluminum oxide grinding processes, key kinetic parameters characterizing the kinetics of particle breakage in a planetary mill were determined. Quantitative data were obtained on the influence of initial particle size, the mass ratio of grinding balls to powder, and the diameter of the grinding media on the rate of reaching a stable particle size.

Using the developed mathematical model, which includes a particle population balance equation with physically grounded breakage and daughter fragment distribution functions, criteria were formulated for selecting optimal grinding regimes to achieve the desired powder characteristics.

Based on the derived functional dependence for the diameter of particles resistant to breakage, process parameters were identified for producing particles with target sizes (from 0.8 to 2 μm).

For example, to obtain aluminum oxide powder (for ceramic matrix composites) with a target particle size of 1.5 μm, the following grinding conditions are recommended: grinding media diameter – 1 mm, mass ratio of grinding media to powder – 3:1.

A software package was implemented in Python to solve the equations of the mathematical model of the grinding process, with the capability to integrate machine learning for refining the energy characteristics of grinding. A digital twin of the process was developed in the Unreal Engine 5 environment, enabling real-time visualization of grinding kinetics and the use of the model as a virtual training module.

The practical significance of the work lies in the applicability of the developed model and software package both for industrial optimization of grinding regimes and for the educational training of specialists in the field of chemical engineering processes and equipment (a software implementation certificate is included in the dissertation appendix).

The provisions submitted for defense:

1. Results of experimental studies on the kinetic patterns of aluminum oxide grinding under various control parameters, such as grinding media size and the mass ratio of grinding media to the material being processed, confirming the attainment of a final constant particle size during prolonged grinding.
2. The structure of thermodynamic driving forces and fluxes for grinding processes.
3. A mathematical model based on the principle of minimum entropy production, allowing the determination of the final particle size resistant to grinding based on the physicochemical properties of materials and grinding conditions.
4. A mathematical model of the kinetics of solid particle grinding in a planetary mill, based on the population balance equation with A and B functions that reflect the actual dynamics of particle breakage (developed from fundamental physicochemical principles).
5. A numerical method for solving the equations of the mathematical model of the grinding process.
6. A software package for simulating grinding processes in a planetary mill.
7. A digital twin of the planetary mill, using the mathematical model as a data source for grinding kinetics, designed for training and conducting computational experiments in a virtual environment.