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ABOUT METHODS OF MODELING THE METAL REFINING PROCESS

ПРО МЕТОДИ МОДЕЛЮВАННЯ ПРОЦЕСУ РАФІНУВАННЯ МЕТАЛУ

This article provides an overview of the main methods used to model the metal refining process, focusing on thermodynamic, kinetic, computational fluid dynamics (CFD) and mathematical models. A mathematical model is considered that takes into account the impulse effect of additives on the melt hydrodynamics in the ladle. The article outlines future directions for improving modeling methods to further improve the efficiency and sustainability of metal refining processes.

***Keywords**: metal refining, review of modeling methods, optimization, efficiency, sustainability.*

Рафінування металу є вирішальним кроком у виробництві високоякісних металів, де домішки видаляються відповідно до певних галузевих стандартів. Процес рафінування включає складні хімічні, фізичні та термодинамічні взаємодії, які відбуваються на різних стадіях, таких як плавлення, окислення та відновлення. Ефективні технології переробки є важливими не лише для покращення якості кінцевого продукту, але й для оптимізації споживання енергії, зменшення відходів та мінімізації впливу на навколишнє середовище.

Через складність цих процесів одних традиційних емпіричних методів часто недостатньо для оптимізації операцій. Тому потреба в точних і прогностичних моделях стала очевидною як в академічних дослідженнях, так і в промислових застосуваннях. Було розроблено різні методи моделювання для імітації процесу переробки, кожна з яких має свої переваги та обмеження. Ці моделі мають на меті надати розуміння поведінки металів і домішок за різних умов, дозволяючи краще контролювати параметри рафінування та підвищувати ефективність процесу.

Стаття містить огляд основних методів, які використовуються для моделювання процесу рафінування металу, зосереджуючись на термодинамічних, кінетичних, обчислювальних гідродинаміках (CFD) і математичних моделях. Кожен метод обговорюється з точки зору його підходу, сильних і слабких сторін. Розглянуто математична модель колективного введення добавок у металеву ванну у ковші. Модель враховує імпульсний вплив добавок на гідродинаміку розплаву, а також перенесення декількох дисперсних фаз. Також у статті окреслено майбутні напрямки вдосконалення цих методів моделювання для подальшого підвищення ефективності та стійкості процесів рафінування металу.

***Ключові слова**: рафінування металу, огляд методів моделювання, оптимізація, ефективність, стійкість.*

Problem's Formulation

Metal refining is a critical step in the production of metals, where impurities are removed to obtain a purer form of the metal. The refining process is essential for improving the quality and properties of metals used in industrial applications, ranging from construction to electronics. The specific refining process depends on the type of metal and the desired level of purity. In general, metal refining can be divided into two main categories: pyrometallurgical and hydrometallurgical processes.

Pyrometallurgical refining involves the use of high temperatures to remove impurities from metals. This method is commonly used for metals such as iron, copper, lead, and zinc. Key pyrometallurgical techniques include smelting, converting, and electrorefining. In the smelting process, ores are heated in a furnace to separate metal from its ore, usually using a reducing agent such as coke. Smelting is often followed by converting, where the molten metal undergoes oxidation to remove sulfur and other impurities.

Electrorefining is another pyrometallurgical technique where impure metal is dissolved in an electrolytic cell, and a purer form of the metal is deposited on the cathode. This method is widely used in the refining of copper and other non-ferrous metals.

The main advantage of pyrometallurgical methods is their efficiency in processing large quantities of metal. However, these methods are energy-intensive and can have significant environmental impacts due to the emission of greenhouse gases and the generation of slag and other by-products.

Hydrometallurgical refining, in contrast, uses aqueous solutions to extract and purify metals from ores. This method is particularly suitable for metals such as gold, silver, uranium, and some rare earth elements. Common hydrometallurgical techniques include leaching, solvent extraction, and electro-winning.

Leaching is a process where a solvent, usually an acid or alkali, is used to dissolve the desired metal from its ore or concentrate. The resulting solution is then processed to recover the metal, either through precipitation, solvent extraction, or electro-winning, where the metal is plated out of the solution onto an electrode.

Hydrometallurgical processes are generally considered more environmentally friendly than pyrometallurgical processes, as they produce fewer emissions and can be performed at lower temperatures. However, these methods can be slower and are often limited by the solubility and reactivity of the metals involved.

In addition to pyrometallurgical and hydrometallurgical methods, other specialized refining techniques may be employed, depending on the metal. For example, zone refining is used for high-purity applications such as the production of semiconductor-grade silicon. This method involves melting a small region of the metal and moving the molten zone along a solid bar, allowing impurities to concentrate in the molten region and be separated from the pure metal.

Another technique, known as vacuum refining, is used for metals that are sensitive to oxidation or contamination, such as titanium and some precious metals. In this process, metal is heated in a vacuum to remove volatile impurities.

Analysis of recent research and publications

The practical guide [1] contains a detailed and systematic overview of both the basic metallurgical and practical engineering aspects of the selection and application of metallic materials. Considers technical properties and applications of steels, cast irons, non-ferrous alloys and metal-matrix composites. The book provides practical information on the technical properties and applications of steels, cast irons, non-ferrous alloys and composites with a metal matrix. Brief reviews and practical implications of metallic structure, imperfections, deformation, and phase transformations are presented. A description of the processes of solidification and casting, recovery, recrystallization and grain growth, and dispersion hardening is provided.

Kinetic modeling of metal processing is presented in work [2]. The article [3] presents achievements in the modeling technique of metal processing. The paper [4] presents present some of the advances in the consideration of the thermochemical and thermophysical properties of metallic materials and slags towards an optimization of the processes. The property models, which developed with respect to the thermodynamics and viscosities of multi-component slags are given. The industrial

application of metal refining models is outlined in article [5]. Prospects of research and further directions of metal purification modeling are given in the article [6].

Formulation of the study purpose

The purpose of this study is to review the main methods of modeling the metal refining process, to study the existing mathematical models describing this process. Identify the strengths and weaknesses of each method. Investigate the application of the considered models in industry, as well as the problems that arise when modeling the metal refining process.

Presenting main material

Modeling techniques for metal refining.

Thermodynamic modeling relies on the laws of thermodynamics, which describe how energy is transferred and transformed in physical systems. Key concepts include Gibbs free energy, enthalpy, and entropy, which are used to assess the feasibility of reactions and phase changes during the refining process. The stability of different phases (solid, liquid, gas) at specific conditions is a fundamental aspect of thermodynamic models.

Common thermodynamic modeling approaches include: equilibrium models, which predict the phase composition at equilibrium based on minimizing the Gibbs free energy; non-equilibrium models, which take into account factors such as reaction kinetics and mass transfer limitations; and phase diagrams, which visually represent the stability of phases with respect to temperature and composition.

Kinetic models are based on the fundamental principles of chemical kinetics, which describe how the rate of a reaction depends on factors such as temperature, concentration of reactants, and the presence of catalysts. These models often use rate equations derived from experimental data to quantify the relationship between these variables [2].

Types of kinetic models: zero-order kinetics - the model assumes that the reaction rate is constant and does not depend on the concentration of the reactants; first-order kinetics - in this model the reaction rate is directly proportional to the concentration of one reactant; second-order kinetics - the model is used when the reaction rate depends on the concentrations of two reactants; complex kinetics.

Computational Fluid Dynamics (CFD) modeling is a sophisticated numerical method employed to analyze and predict fluid flow behavior and its interaction with solid structures in metal refining processes. This approach utilizes computational algorithms and simulations to solve the governing equations of fluid dynamics, primarily the Navier-Stokes equations, which describe the motion of viscous fluid substances.

CFD involves discretizing the fluid domain into a mesh, where the governing equations are solved at each mesh point. The choice of mesh type (structured vs. unstructured) can significantly influence the accuracy and computational efficiency of the simulation.

Mathematical modeling involves formulating mathematical equations that represent the physical and chemical phenomena occurring during purification. These models can vary in complexity from simple empirical equations to complex multiparameter modeling.

Advantages and limitations of modeling methods.

One of the primary advantages of *thermodynamic models* is their ability to provide insights into phase equilibria. By calculating phase diagrams, these models enable researchers to identify stable and metastable phases of metal alloys and impurities during refining. This knowledge is essential for selecting appropriate processing conditions to achieve the desired purity and yield of the final metal product.

Thermodynamic models also allow for the evaluation of reaction equilibria.

However, thermodynamic models also have limitations. One significant drawback is that they often rely on idealized assumptions, such as the behavior of gases and liquids as ideal mixtures. Another challenge is the availability of reliable thermodynamic data for various metal systems. In many cases, the necessary data may be incomplete or only available for certain temperature and pressure ranges, limiting the applicability of the models. Consequently, the use of thermodynamic models often requires supplementary experimental validation to ensure their reliability and accuracy.

Kinetic models play a critical role in understanding and optimizing the metal refining process, as they focus on the rates of chemical reactions and the factors influencing these rates.

The advantages of kinetic models include: the ability to predict, optimize processes, and expand. The limitations of kinetic models include: their complexity; assumptions that may not correspond to real conditions; and limited scope of application.

The advantages of CFD models are detailed flow visualization, optimization of operating conditions, reduced experimental costs, integration with other modeling methods. Limitations of CFD models: computational intensity, modeling complexity, verification requirements, user expertise.

Mathematical models play a crucial role in the process of metal refining by providing a framework for understanding and predicting the behavior of various refining processes. These models utilize mathematical equations to represent the relationships between different variables involved in metal extraction and purification.

The advantages of mathematical modeling are predictability, cost-effectiveness, and integration with computational tools. The limitations of mathematical modeling include model assumptions, data dependence, complexity, and calibration.

Each modeling technique offers unique advantages and limitations, making them suitable for different aspects of the metal refining process. A combined approach, leveraging the strengths of multiple modeling techniques, may often yield the most comprehensive understanding of the metal refining process.

The application of modeling techniques in the metal refining industry plays a crucial role in optimizing processes, enhancing product quality, and improving operational efficiency. Various modeling approaches are employed across different stages of metal refining, each serving distinct purposes that contribute to overall productivity and sustainability [5].

Challenges and future directions.

The modeling of metal refining processes faces several challenges that can impact the accuracy and applicability of the models developed. Understanding these challenges is crucial for advancing research and improving industrial practices [6].

One significant challenge is the complexity of metal refining processes themselves. These processes often involve a multitude of variables, including temperature, pressure, chemical compositions, and reaction kinetics. Capturing the intricate interactions among these variables in a model can be difficult, leading to simplifications that may not accurately reflect real-world conditions. For example, thermodynamic models may struggle to account for non-ideal behavior in multi-component systems, which can result in discrepancies between predicted and actual outcomes.

Another challenge is the integration of data from various sources. Effective modeling requires high-quality data on material properties, reaction rates, and environmental conditions. However, discrepancies in data collection methods, variations in experimental setups, and differences in material purity can hinder the development of robust models. Furthermore, there is often a lack of standardized data across different studies, making it difficult to compare results or validate models.

Computational limitations also pose a challenge. While advancements in computational power have enabled more sophisticated modeling techniques, the computational cost associated with high-fidelity simulations, such as those using Computational Fluid Dynamics (CFD), can be prohibitive. This limitation often forces researchers to balance model complexity with computational feasibility, potentially leading to less accurate representations of the refining process.

Looking ahead, there are several promising directions for future research in metal refining process modeling. One approach is the incorporation of machine learning techniques to enhance model accuracy and predictive capabilities. By leveraging large datasets from experimental and operational data, machine learning can help identify patterns and optimize parameters that traditional modeling approaches may overlook.

Additionally, the development of hybrid models that combine various modeling techniques—such as integrating kinetic and thermodynamic models with CFD—can provide a more comprehensive understanding of the refining processes. These hybrid models can capitalize on the strengths of each method while mitigating their individual weaknesses, leading to improved predictive power.

Moreover, advancements in experimental techniques, such as in-situ monitoring and advanced imaging, can provide valuable data to refine existing models. By continuously updating models with

real-time data, researchers can enhance their accuracy and reliability, making them more applicable to industrial settings.

In conclusion, while the modeling of metal refining processes presents numerous challenges, the integration of advanced computational techniques, machine learning, and improved experimental data collection holds promise for overcoming these obstacles.

The mathematical model presented in [7] was chosen for the study. This model takes into account the effective compressibility of the medium, mutual movement, interaction and transformation of several phases: melt; gas, which is captured when adding additives and by a metal jet; solid finely dispersed phase of modifying materials; liquid dispersed phase of the products of their dissolution or melting, and other phases into which it passes.

The main assumptions of the mathematical model: phase transformations of the gas phase α are neglected; when additives are introduced into the ladle, as well as when the melt jet enters the surface of the melt (during filling), air is trapped; we neglect the collective component of the velocity of liquid dispersed phases η_l relative to the melt; we neglect the heat spent on heating the inert gas.

The hydrodynamics of the environment as a whole and the mass transfer of the gas phase are described by the following system of equations [8]:

$$\frac{d\vec{v}}{dt} = -\vec{\nabla}\tilde{p} + \upsilon_e \Delta\vec{v} - [\alpha + (1-x)\beta]\vec{g} + \vec{f}\,; \tag{1}$$

$$\vec{\nabla}\cdot\vec{v} = \psi_a + \psi_b\,; \tag{2}$$

$$\frac{\partial\alpha}{\partial t} + \vec{\nabla}\cdot\left[\alpha\left(\vec{v} + \vec{w}_a^c\right)\right] = \vec{\nabla}\cdot\left(D_a\vec{\nabla}\alpha\right) + \psi_a\,; \tag{3}$$

$$\frac{\partial\beta}{\partial t} + \vec{\nabla}\cdot\left[\beta\left(\vec{v} + \vec{w}_b^c\right)\right] = \vec{\nabla}\cdot\left(D_b\vec{\nabla}\beta\right) + \psi_b\,, \tag{4}$$

where $\vec{v}$ — barycentric velocity of the medium; t — process time, $\tilde{p}$ — dynamic component of pressure normalized to the true density of the melt; $\upsilon_e = \upsilon + \Delta l\,|v|/\mathrm{Re}_\Delta$ — effective coefficient of turbulent kinematic viscosity in a two-parameter turbulence model with parameters: υ — isotropic effective viscosity and Re_Δ — by grid Reynolds number on a grid with characteristic pitch Δl; $\vec{g}$ — acceleration of free fall; α and β – coefficient of volumetric gas diffusion and bulk density of the solid phase (lump materials) in the medium; x – the ratio of the true densities of the solid dispersed phase and the steel melt; D_a — effective turbulent diffusion coefficients of the gas phase; D_b – effective turbulent diffusion coefficients of the solid phase; ρ_0 – true melt density; $\vec{f}$ — volumetric density of forces arising from the action of the flow of additives introduced into the ladle; ψ_a and ψ_b — bulk densities of sources of gas and solid dispersed phases that arise as a result of the supply of gas and impurity materials into the volume of the ladle; $\vec{w}_a^c$ and $\vec{w}_b^c$ — collective velocities of the gas and solid phases.

In the calculations we accept: $D_a = D_b = \upsilon_e$.

The heat transfer process is described by the equation [7]:

$$C_r\frac{dT}{dt} = \vec{\nabla}\cdot\left(\lambda_e'\vec{\nabla}T\right) + \theta\,, \tag{5}$$

where T — temperature, θ – source determined by thermal effects of initial heating of impurities and phase transformations. This component is specified when considering individual processes. C_r and λ_e' are effective coefficients that take into account the presence of dispersed phases in the melt and are determined by the formulas given in [7].

Equations (1)—(4) are solved numerically by the method of splitting by physical factors for non-solenoid motion of multiphase media [7]. As a result of the assumptions made, we arrive at a three-stage calculation scheme:

I $\quad \tilde{\tilde{\vec{v}}} = \vec{v}^n + \tau\{\upsilon_e \Delta \vec{v} - [\alpha + (1-x)\beta]\vec{g} + \vec{f}\}^n$,

II $\quad \Delta \tilde{p} = (\vec{\nabla} \cdot \tilde{\tilde{\vec{v}}} - \psi_a - \psi_b)/\tau$,

III $\quad \vec{v}^{n+1} = \tilde{\tilde{\vec{v}}} - \tau \vec{\nabla} \tilde{p}$,

$$\alpha^{n+1} = \alpha^n - \tau\{\vec{\nabla} \cdot [\alpha\ (\vec{v} + \vec{w}_a^c)] - \vec{\nabla} \cdot (D_a \vec{\nabla} \alpha) + \psi_a\}^n,$$

$$\beta^{n+1} = \beta^n - \tau\{\vec{\nabla} \cdot [\beta\ (\vec{v} + \vec{w}_b^c)] - \vec{\nabla} \cdot (D_b \vec{\nabla} \beta) + \psi_b\}^n.$$

Here τ — step by time, n — time layer number, a $\tilde{\tilde{\vec{v}}}$ — intermediate velocity, which is calculated without taking into account the pressure field.

Equation (5) will be solved using the explicit difference scheme.

This scheme is implemented in three-dimensional space in cylindrical coordinates on a uniform checkerboard grid.

The boundary conditions for the calculated quantities on the solid surfaces of the bucket, the axis of symmetry and the metal mirror are set in a standard way inherent in the method of splitting by physical factors when using a checkerboard grid [7].

The location on the surface mirror of the metal where the additives are introduced is selected as follows. Let S_m be the surface area of the melt to which the additives are supplied, and $\vec{V}_m$ be the rate of uniform distribution of the additives over the area by perpendicular to the surface.

Then the value of the barycentric velocity of the melt surface $\vec{v}_m$, taking into account the momentum $\mu V_m = (v_m S_m \rho) v_m$ transferred from the additive stream to the melt volume per unit time, can be found using the formula:

$$v_m = \sqrt{\mu V_m / (S_m \rho)}. \quad (6)$$

Here ρ — density of the medium, and $(v_m S_m \rho)$ – mass flow of the medium through the surface S_m.

By setting the velocity $\vec{v}_m$ on the surface S_m as the limiting one, we thereby take into account the force factor $\vec{f}$ of the influence of the additive jet on the hydrodynamics of the melt in the ladle, which appears in equation (1).

The boundary conditions for the bulk density β of the solid dispersed phase on the surface S_m through which the additives are introduced are set based on the law of conservation of mass: $\mu = \beta_m \rho_b^0 v_m S_m$, where β_m is the value on the surface S_m [8]:

$$\beta_m = \mu / (\rho_b^0 v_m S_m). \quad (7)$$

Such a boundary condition assignment for β will allow taking into account the volumetric source ψ_b of the solid dispersed phase, which appears in equations (2) and (4).

Conclusions

The modeling of metal refining processes is an essential aspect of modern metallurgy, facilitating the optimization of operations, the enhancement of product quality, and the reduction of environmental impact. The various modeling techniques — thermodynamic, kinetic, computational fluid dynamics (CFD), and mathematical modeling — each offer unique advantages and limitations that can influence their applicability in different scenarios.

The mathematical model presented in the paper is based on the method of collective description of the dynamics of solid dispersed phases [8]. Using this model, it is possible to calculate the hydrodynamics of the melt taking into account the influence of solid additives fed into the ladle at the stage of out-of-furnace steel processing.

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