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O.O. Kuzyk, V.M. Atamanyuk, Y.M. Gumnitsky, O.S. Ivashchuk

INTENSIFICATION OF MASS TRANSFER DURING THE DISSOLUTION OF AMMONIUM TETRAFLUOROBORATE BY MECHANICAL STIRRING

Lviv Polytechnic National University, Lviv, Ukraine

Ammonium tetrafluoroborate (ATFB) is a versatile chemical compound widely utilized in agriculture, disinfection, and chemical synthesis. This study investigates the intensification of mass transfer during the dissolution of ATFB in a «solid–liquid» system facilitated by mechanical stirring. The primary objective was to determine mass transfer patterns to optimize reactor design and improve energy efficiency in industrial applications. Experiments were conducted using spherical ATFB particles in a cylindrical vessel equipped with a three-blade impeller. The dissolution kinetics was examined across a temperature range of 293–323 K and impeller rotation frequencies of 1.67–6.67 s^{-1}. The results demonstrated that both temperature and rotation frequency significantly influence the rate of surface area reduction and dissolution intensity. Specifically, increasing the temperature from 293 K to 323 K resulted in a 2.58-fold increase in dissolution intensity, while increasing rotation frequency from 1.67 s^{-1} to 6.67 s^{-1} yielded a 1.9-fold increase. Analysis of the mass transfer coefficients indicated that the dissolution process operates in a diffusion-controlled regime. To generalize the experimental data, a dimensionless empirical correlation for the Sherwood number was derived: $Sh=5.8\cdot Re^{0.5}\cdot Sc^{0.33}d_p/D_a$. The proposed model aligns with experimental results with a maximum absolute relative error of less than 6%, confirming its adequacy for engineering calculations and the prediction of ATFB dissolution rates in industrial reactors.

Keywords: ammonium tetrafluoroborate, dissolution kinetics, mass transfer intensification, mechanical stirring, Sherwood number, solid–liquid system, mass transfer coefficient.

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Introduction

Ammonium tetrafluoroborate (ATFB) is a chemical compound that possesses properties facilitating its application across various industries. It exhibits significant biological activity as a pesticide in agriculture [1], is utilized in the production of disinfectants for equipment and facilities [2], and serves as a reagent in the synthesis of novel chemical compounds [3].

Due to their specific properties, boron-containing compounds are essential components of many micronutrient fertilizers. The demand for fertilizers in the agrarian sector has been steadily increasing in recent years due to the phenomenon known as «soil depletion» [4]. Furthermore, due to the full-scale invasion and economic factors, fertilizer usage in Ukraine has undergone significant changes. The general trend indicates a reduction in fertilizer application by approximately 50% compared to the pre-war year of 2021. The analysis in ref. [5] reveals a sharp decline in consumption in 2022 by 50–70% due to logistical

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difficulties and the loss of warehouses; in 2023, fertilizer use decreased by 3754% compared to 2021. As of 2024, the market has stabilized at the level of 3.2 million tons. A significant dependence on imports is observed, particularly regarding ammonium sulfate (the expected import volume is 500 thousand tons). Domestic production is constrained by energy supply issues. Considering the aforementioned factors, fertilizer use efficiency is a critical issue. Granulation enables a substantial reduction in the product's tendency to caking, thereby simplifying storage, transportation, and dosing [6]. The application of granular fertilizers is critical for precise local application and the controlled, prolonged release of nutrients into the soil. This ensures stable plant nutrition throughout the growing season. Conversely, liquid solutions derived from or based on them allow for the rapid adsorption of nutrients through the leaf surface (foliar feeding) or via drip irrigation systems, ensuring immediate correction of nutrient deficiencies and enhancing their assimilation efficiency of plants. Substances in granular form possess superior physicochemical characteristics compared to powder forms [7]. On the other hand, according to the findings in [8], ATFB exhibits high anion toxicity upon hydrolysis, resulting in the formation of fluorine ions that are harmful to the environment [9]. Therefore, minimizing ATFB dust formation during storage, transportation, and dosing is a pressing issue, which in turn confirms the relevance of utilizing the granular form of fertilizers.

ATFB is applied in industry as an aqueous solution [10]. Dissolution is considered a spontaneous diffusion-kinetic process occurring during the interaction of the solute and solvent in a «solid–liquid» system.

Designing reactors for «solid–liquid» systems requires the consideration of various parameters, specifically the kinetic and hydrodynamic characteristics of the reactors. The overall process rate is determined by the chemical reaction kinetics and the physical mechanisms of mass transfer between the liquid and solid phases. Consequently, the development of such reactors requires determined mass transfer parameters.

The mass transfer process between the solid phase and liquid is the subject of research in various reactor types. However, as noted by the authors in [11], research on the mass transfer coefficient at the «solid–liquid» interface significantly lags behind research on gas–liquid mass transfer in multiphase reactors.

Mechanically stirred two-phase («solid–liquid») and three-phase («gas–solid–liquid») reactors belong to the primary class of multiphase reactors. Due to their reliability and practicality, they are extensively employed in the chemical industry [11].

One of the key reasons for applying mechanical stirring is to ensure the maximum mass transfer surface area [12].

Research results available in the literature have been based on determining the mass transfer coefficient in «solid–liquid» stirred reactors using one of the following approaches: dimensional analysis, isotropic turbulence theory, and slip velocity theory [11].

Correlations based on dimensional analysis are simple to use; however, they do not account for the specific influence of various system parameters on the «solid-liquid» mass transfer coefficient. Such correlations are applicable only to configurations that possess geometric similarity and operate within the same parameter range, such as the Reynolds number.

Isotropic turbulence theory assumes that at the same specific power input, the value of the «solid–liquid» mass transfer coefficient is independent of the geometric configuration and differences in the liquid phase density. However, experimental results obtained in ref. [13] show that while this theory reliably reflects the general trend of mass transfer coefficient variation with changes in energy input, it does not yield a universal correlation for different geometric configurations and a wide range of Schmidt numbers. Thus, using correlations based on isotropic turbulence theory to predict the mass transfer coefficient in «solid–liquid» mechanically stirred reactors with distinct geometric configurations may lead to inaccurate results.

Studies aimed at establishing the relationship between the «solid–liquid» mass transfer coefficient and the effective slip velocity of the particle relative to the liquid are crucial for better prediction of the mass transfer process. However, for large-scale reactors, there is a lack of research data regarding the determination of the mass transfer coefficient in turbulent solvent flow, and the complexity of solving nonlinear equations of particle motion in turbulent flow complicates the determination of a representative slip velocity.

The dissolution of sparingly soluble substances in liquids is a rather time-consuming and labor-intensive process [14].

Various methods are employed to accelerate the dissolution process: direct flow around material particles, dissolution in a state of particle suspension, dissolution under conditions of rotational liquid motion [13], as well as dissolution with periodic changes in liquid flow direction and velocity associated with particle inertia using ultrasound [14]. The most common method for intensifying the dissolution process is mechanical stirring, typically achieved using an agitator.

Modern methods for investigating dissolution during mechanical stirring [15] are based on dissolving a powdered substance in water [16] or a solid body suspended at a specific height within the reactor [17]. Currently, the study [18] explaining mass transfer processes between an ensemble of freely moving spherical solid particles in a reactor and a solvent [19] is highly relevant, given the need to optimize and increase the efficiency of chemical and biochemical reactors, where the rate of the final process is often limited specifically by the rate of interfacial mass transfer at the particle surface. Such processes are widespread in industrial mixing apparatuses. Therefore, determining mass transfer patterns is a pressing task, including for practical reasons. Implementing the research results obtained will significantly improve energy efficiency and product quality, which in turn will influence the cost of the finished product.

Experimental

The experimental setup, along with a detailed description of its operating principle and the methodology used in this study, aligns with previously published methodologies and is comprehensively described in works [18,19] (Fig. 1).

Chemically pure ammonium tetrafluoroborate was used in the study. The experiment was conducted in a cylindrical vessel with a height of 0.21 m and a diameter of 0.16 m. The temperature was controlled using a SESTOS D1S-VR-220 controller and a UNI-T UT-T03 thermocouple with an accuracy of 0.5 K. An AD3000 electronic balance with an accuracy of $0.1\cdot10^{-4}$ kg was used to measure the mass of the spheres. The diameter of the spheres was measured using a YT-72300 micrometer with an accuracy of $0.1\cdot10^{-4}$ m. The described instruments and measurement methods ensured the stability and reproducibility of the experimental conditions.

To proceed to the sample preparation stage, it was necessary to obtain solid particles of a specified geometric shape. Based on the results of preliminary pilot studies, the compaction pressure value was tested and determined to ensure the formation of spheres with minimal deviations in material structure and porosity. ATFB powder was loaded into a mold, and spheres with a diameter of 20 mm were pressed at a pressure of 4 MPa, yielding samples uniform in size and resistant to mechanical impact. After formation, the ammonium tetrafluoroborate spheres (ATFBS) were immersed in a container with a saturated ATFB solution. At specific time intervals, the spheres were removed, surface moisture was removed using filter paper, and their diameter and mass were measured. The experiment continued until the spheres reached a constant mass, indicating that their saturation process was complete.

To experimentally investigate the dissolution kinetics of ATFBS, the heating element was switched on, and distilled water in the cylindrical vessel was heated to the specified temperature. The rotation of the three-blade impeller was activated at a set frequency, and 5 ATFBS were simultaneously loaded. Every 180 seconds, the spheres were removed from the container, surface moisture was removed using filter paper, and the diameter and mass of the spheres were measured. Each experiment was repeated at least three times until stable values were obtained. The change in ammonium tetrafluoroborate concentration was calculated based on the change in ATFBS mass, and the ATFBS surface area was determined by measuring

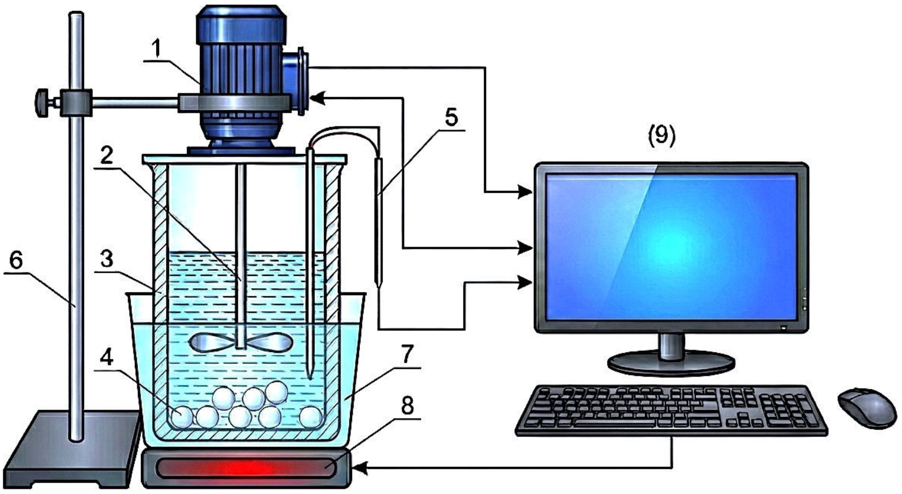


Fig. 1. Experimental setup: 1 – asynchronous motor; 2 – three-blade impeller; 3 – cylindrical vessel; 4 – ATFB spheres; 5 – thermocouple; 6 – support stand; 7 – water bath; 8 – heating element; 9 – computer-integrated system

its diameter. The experiments were conducted at temperatures of 293, 303, 313, and 323 K, and impeller rotation frequencies of 1.67, 3.33, 5, and 6.67 s^{-1}.

The physical characteristics of ATFB and the ammonium tetrafluoroborate solution, as per reference data [20], are presented in Tables 1 and 2.

The research methodology employed in this study has been successfully validated and utilized in a series of our previous studies, specifically in publications [18,19]. This prior application facilitated the establishment of key concepts, the mathematical framework, and empirical correlations that form the basis of the current work. Building upon this methodological foundation, we established a basis for the further investigation of complex hydrodynamic and mass transfer phenomena.

To generalize the experimental data and evaluate the efficiency of convective mass transfer, the dimensionless Sherwood number (*Sh*) was utilized. The Sherwood number represents the ratio of convective mass transfer to mass transfer driven solely by molecular diffusion. Its application enables the generalization of results obtained across different scales and using various substances, as well as the expression of the mass transfer coefficient (β) as a function of hydrodynamic conditions (Reynolds number, *Re*), the physical properties of the system (Schmidt number, *Sc*), and the geometric simplex (Γ):

$$Sh=f\left(Re,Sc,\Gamma\right).$$

In this study, we focused on determining the empirical correlation of the Sherwood number for a particle ensemble, thereby establishing a foundation for predicting the dissolution process rate in industrial reactors.

The empirical equation for determining the Sherwood number for the system under investigation is expressed as follows:

$$Sh=A\cdot Re^{x}\cdot Sc^{y}\cdot\Gamma, \qquad (1)$$

where A is the proportionality constant determined based on experimental data.

The Reynolds number, which characterizes the system hydrodynamics, was calculated as follows:

$$Re=\frac{\rho\cdot n\cdot d_m^2}{\mu}, \qquad (2)$$

where ρ is the liquid density (kg/m^3); *n* is the impeller rotation frequency (s^{-1}); *d* is the three-blade impeller diameter (m); μ is the liquid dynamic viscosity (Pa·s).

The Schmidt number, which characterizes the physical parameters of the system, was calculated as follows:

$$Sc=\frac{\nu}{D}, \qquad (3)$$

where ν is the solution kinematic viscosity (m^2/s).

The geometric simplex value was determined as the ratio of the particle diameter to the apparatus diameter:

$$\Gamma=\frac{d_p}{D_a}, \qquad (4)$$

where d_p is the ATFBS diameter (m); D_a is the apparatus diameter (m).

Considering that the physical parameters of the solution vary within a narrow range, and in accordance with the recommendations [21], the exponent for the Schmidt number was assumed to be 0.33. Thus, the empirical equation takes the form:

$$Sh=A\cdot Re^{x}\cdot Sc^{0.33}\cdot\Gamma. \qquad (5)$$

The diffusion coefficient was estimated using

Table 1

Physical characteristics of ammonium tetrafluoroborate spheres

Diameter, $d\cdot10^3$, m	Mass, $M_0\cdot10^3$, kg	Porosity, ε, %	Volume, $V\cdot10^6$, m^3	Area, $F\cdot10^3$, m^2	Molar mass, kg/mol
20	6.5	12	4.19	1.256	104.84

Table 2

Saturation concentration, dynamic viscosity, and density of the ammonium tetrafluoroborate solvent at different temperatures

T, K	293	303	313	323
Cs, kg/m^3	25	31	37	43
$\mu\cdot10^4$, Pa·s	10.04	7.97	6.58	5.47
ρ, kg/m^3	998.20	995.60	992.24	988.00

the Wilke-Chang method via the following equation [22]:

$$D=7.4\cdot10^{-8}\cdot\left[\frac{\left(\phi\cdot M_p\right)^{0.5}\cdot T}{\mu_p\cdot V_1^{0.6}}\right]. \qquad (6)$$

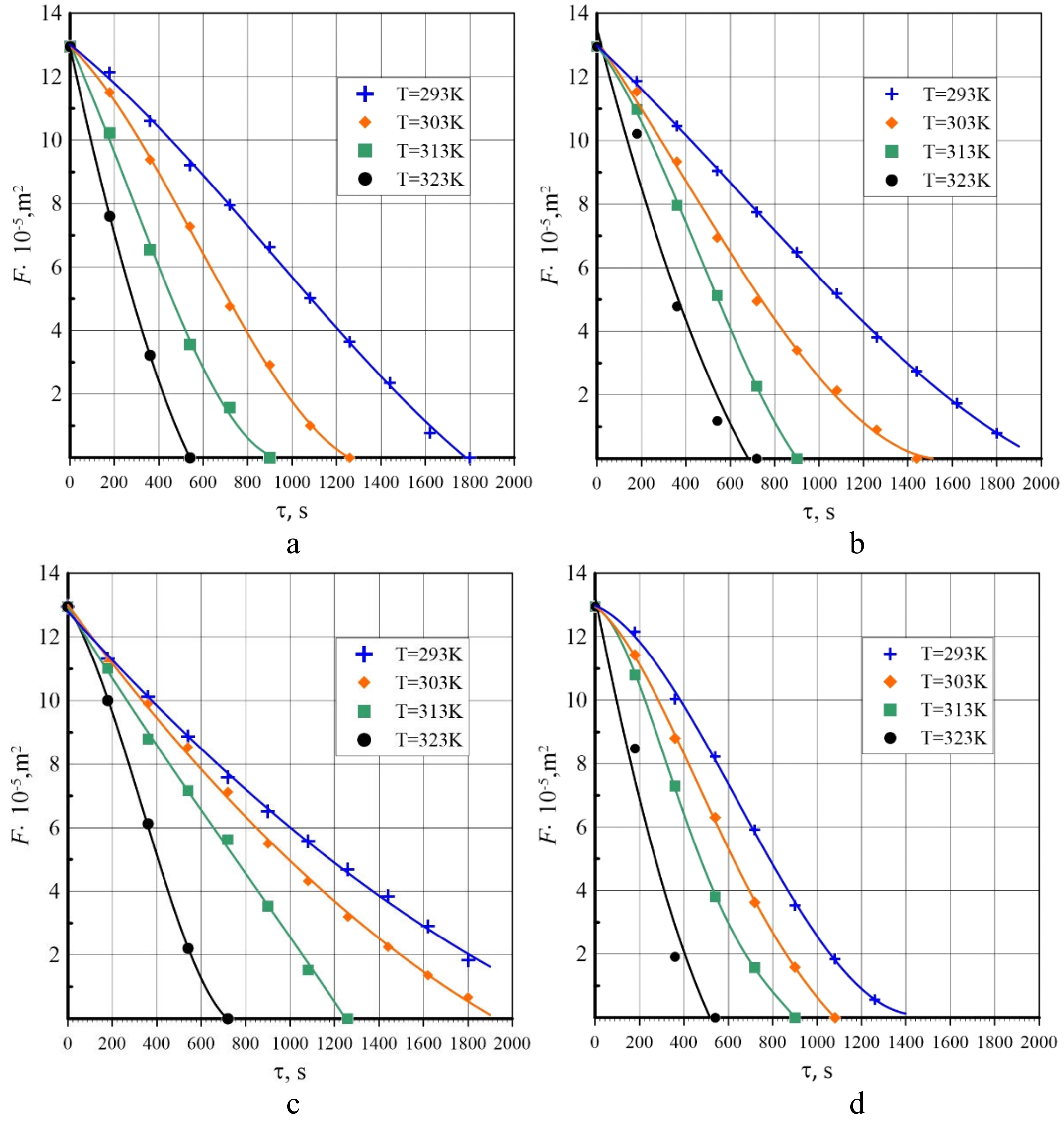
where D is the mutual diffusion coefficient at infinite dilution of the solute (m^2/s); M_p is the molar mass of the solvent (kg/kmol); T is the temperature (K); μ_p is the solvent viscosity (mPa·s); V_1 is the molar volume of the solute at its boiling point (m^3/mol); ϕ is the solvent «association parameter» (for water ϕ=2.6 [22]).

Results and discussion

Figure 2 presents the experimental results illustrating the reduction in the diameter of ammonium tetrafluoroborate spheres (ATFBS) caused by their dissolution. Given that the mass transfer surface area is not constant, an approach involving the calculation of the average surface area of the spheres for each combination of solution temperature and impeller rotation frequency was employed to ensure precise determination and accurate data processing.

The analysis of the experimental results regarding the change in ATFBS surface area, presented in Fig. 2, indicates that the rate of reduction of the average sphere surface area is influenced by both the impeller rotation frequency and the temperature of the distilled water (Table 3).

For example, within 600 s, at a rotation frequency of 1.67 s^{-1} and a temperature of 293 K, the average



a b c d

Fig. 2. Variation in the average surface area of ATFBS during dissolution: a – 1.67 s^{-1}; b – 3.33 s^{-1}; c – 5 s^{-1}; d – 6.67 s^{-1}

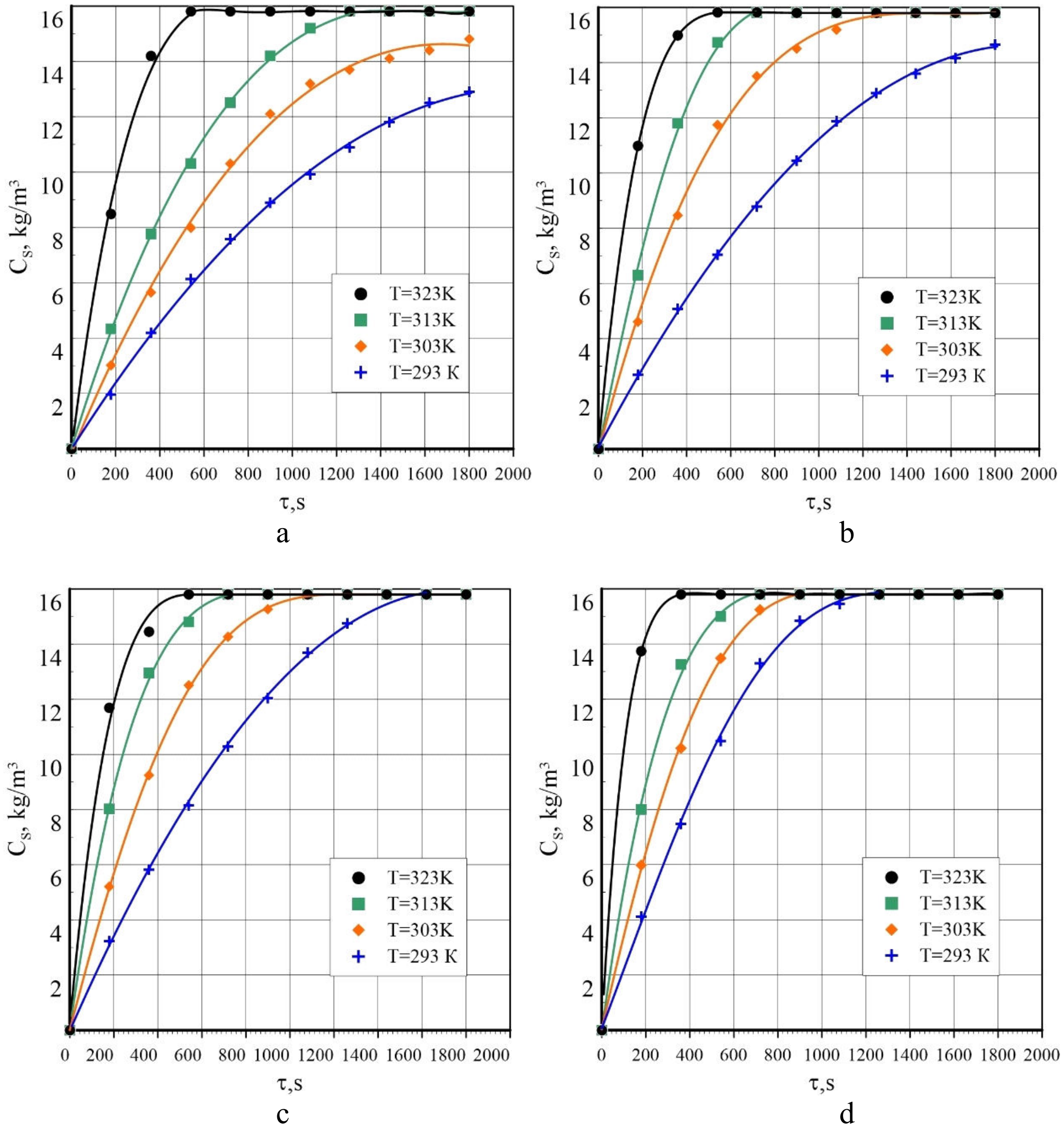
sphere surface area decreases from $1.30\cdot10^{-3}$ m^2 to $0.85\cdot10^{-3}$ m^2, i.e., by a factor of 1.52. At a temperature of 323 K and a rotation frequency of 1.67 s^{-1}, it decreases to $0.17\cdot10^{-3}$ m^2, i.e., by a factor of 7.65.

At an impeller rotation frequency of 5 s^{-1} and a temperature of 293 K over 600 s, the average sphere surface area decreases from $1.30\cdot10^{-3}$ m^2 to $0.84\cdot10^{-3}$ m^2, i.e., by a factor of 1.53, whereas at a temperature of 323 K, it decreases to $0.07\cdot10^{-3}$ m^2, i.e., by a factor of 18.57.

As illustrated in Fig. 3, the ATFB solution concentration increases correspondingly. Notably, at an impeller rotation frequency of 1.67 s^{-1}, increasing the water temperature from 293 to 323 K over 600 s results in a 2.58-fold increase in dissolution intensity. Furthermore, at a temperature of 323 K, changing the impeller rotation frequency from 1.67 s^{-1} to 6.67 s^{-1} results in a 1.9-fold increase in dissolution intensity.

To generalize the experimental data, it is appropriate to present them in the form of dimensionless groups. Such a representation of experimental results enables their application for predicting the dissolution kinetics of ATFBS in industrial reactors of various volumes.

The ratio of mass transfer coefficients corresponding to a temperature difference of 10 K indicates a variation within the range of 1.04–1.26. This suggests that the process operates in the diffusion-controlled regime within the investigated range.



a

b

c

d

Fig. 3. Dissolution kinetics of ATFBS: a – 1.67 s^{-1}; b – 3.33 s^{-1}; c – 5 s^{-1}; d – 6.67 s^{-1}

The calculated values of the internal diffusion coefficients of ammonium tetrafluoroborate from the sphere pores into the solution and the Schmidt numbers, as a function of the solution temperature, are presented in Table 4.

To determine the unknown coefficients A and x in Equation (1), the experimental data were presented as a graphical dependence: $Sh/Sc=f(Re)$ in logarithmic coordinates (Fig. 4).

By approximating the experimental results with a power function, the calculated values of coefficients A and x were obtained for the investigated ammonium tetrafluoroborate solution temperatures:

$$Sh=5.8\cdot Re^{0.5}\cdot Sc^{0.33}\cdot\frac{d_p}{D_a}. \qquad (7)$$

A comparison of the Sherwood numbers calculated based on experimental data with the theoretical values obtained using Eq. (7) is presented in Fig. 4. The maximum absolute relative error does not exceed 6%, which is considered acceptable for practical calculations of the technological parameters for ATFBS dissolution in chemical industry enterprises.

Conclusions

The significant influence of the solution temperature and impeller rotation frequency on the rate of reduction of the average sphere surface area has been established. The increase in ATFB solution concentration corresponds to the intensity of the sphere surface reduction, confirming a direct relationship between the heat and mass transfer conditions and the dissolution rate.

Table 3

Averaged values of mass transfer coefficients and ATFBS diameters as a function of temperature and impeller rotation frequency over 1800 s

n, s^{-1}	$\beta\cdot10^4$, m/s				$d_k\cdot10^2$, m			
	293 K	303 K	313 K	323 K	293 K	303 K	313 K	323 K
1.67	2.26	2.80	3.06	3.51	1.36	1.37	1.50	1.59
3.33	3.22	3.78	4.14	5.14	1.30	1.37	1.60	1.48
5	3.59	4.42	5.57	5.75	1.45	1.46	1.42	1.61
6.67	4.40	5.20	5.68	6.57	1.41	1.42	1.56	1.57

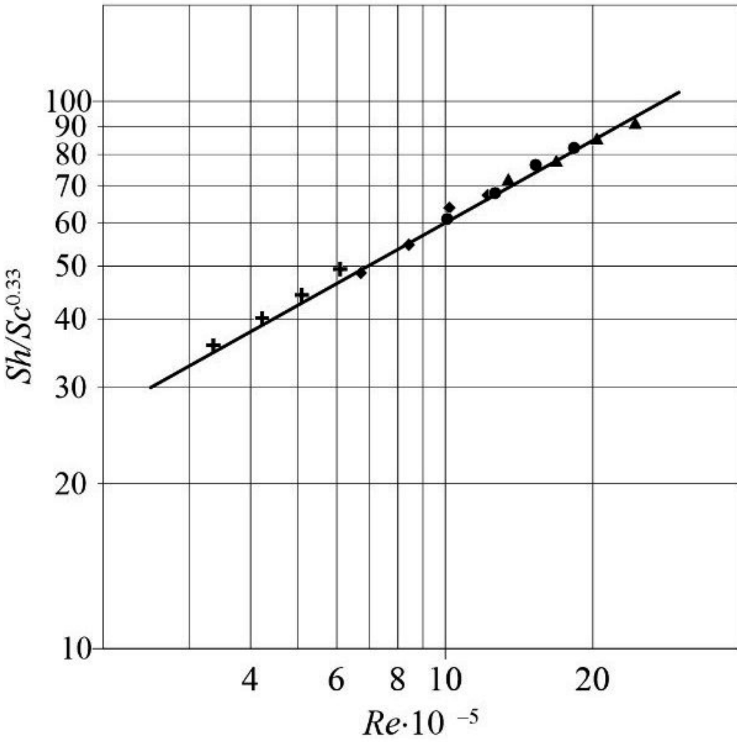


Fig. 4. Graphical dependence of $Sh/Sc^{0.33}$ based on experimental data (symbols +, ♦, Δ, •) and theoretically calculated values (solid line) as a function of the Reynolds number

Table 4

Values of ammonium tetrafluoroborate internal diffusion coefficients and Schmidt numbers

T, K	$D \cdot 10^8$ m^2/s	Sc
293	2.55	39.30
303	3.22	24.10
313	4.15	15.96
323	5.16	10.73

It has been established that the dissolution process of ammonium tetrafluoroborate spheres occurs in the diffusion-controlled regime. This is confirmed by the ratio of mass transfer coefficients for a temperature difference of 10 K, the value of which lies within the range of 1.04–1.26 for the investigated temperature interval.

By approximating the experimental data with a power dependence, calculated values of the coefficients characterizing the influence of solution temperature on the mass transfer kinetics during ATFBS dissolution were obtained. The maximum absolute relative error between the experimentally and theoretically obtained Sherwood number values does not exceed 6%. This indicates the adequacy of the correlation used and allows its application for engineering calculations of ATFBS dissolution process parameters under industrial conditions.

The obtained results enable the prediction of the ATFBS dissolution rate under various hydrodynamic and temperature conditions, which is crucial for optimizing technological processes in the chemical industry.

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ІНТЕНСИФІКАЦІЯ МАСООБМІНУ ПІД ЧАС РОЗЧИНЕННЯ АМОНІЙ ТЕТРАФТОРОБОРАТУ ЗА УМОВ МЕХАНІЧНОГО ПЕРЕМІШУВАННЯ

О.О. Кузик, В.М. Атаманюк, Я.М. Гумницький, О.С. Іващук

Амоній тетрафтороборат (АТФБ) є багатофункціональною хімічною сполукою, що широко використовується у сільському господарстві, дезінфекції та хімічному синтезі. Це дослідження присвячене вивченню інтенсифікації масообміну під час розчинення АТФБ у системі «тверде тіло–рідина» за умов механічного перемішування. Основною метою роботи було визначення закономірностей масообміну для оптимізації конструкції реакторів та підвищення енергоефективності у промислових застосуваннях. Експерименти проводили з використанням сферичних частинок АТФБ у циліндричному апараті, обладнаному трилопатевою мішалкою. Кінетику розчинення досліджували в діапазонах температур 293–323 K та частот обертання мішалки 1,67–6,67 $с^{-1}$. Результати показали, що як температура, так і частота обертання суттєво впливають на швидкість зменшення площі поверхні та інтенсивність розчинення. Зокрема, підвищення температури з 293 K до 323 K привело до збільшення інтенсивності розчинення у 2,58 рази, тоді як збільшення частоти обертання з 1,67 $с^{-1}$ до 6,67 $с^{-1}$ забезпечило зростання у 1,9 рази. Аналіз коефіцієнтів масовіддачі показав, що процес розчинення протікає в дифузійній області. Для узагальнення експериментальних даних було отримано безрозмірне критеріальне рівняння для числа Шервуда: $Sh=5{,}8\cdot Re^{0{,}5}\cdot Sc^{0{,}33}\cdot d_p/D_a$. Запропонована модель узгоджується з експериментальними результатами з максимальною відносною похибкою менше 6%, що підтверджує її адекватність для інженерних розрахунків та прогнозування швидкості розчинення АТФБ у промислових реакторах.

Ключові слова: амоній тетрафтороборат; кінетика розчинення; інтенсифікація масообміну; механічне перемішування; число Шервуда; система тверде тіло–рідина; коефіцієнт масообміну.

INTENSIFICATION OF MASS TRANSFER DURING THE DISSOLUTION OF AMMONIUM TETRAFLUOROBORATE BY MECHANICAL STIRRING

O.O. Kuzyk *, V.M. Atamanyuk, Y.M. Gumnitsky, O.S. Ivashchuk

Lviv Polytechnic National University, Lviv, Ukraine

*** e-mail: oleksandr.o.kuzyk@lpnu.ua**

Ammonium tetrafluoroborate (ATFB) is a versatile chemical compound widely utilized in agriculture, disinfection, and chemical synthesis. This study investigates the intensification of mass transfer during the dissolution of ATFB in a «solid–liquid» system facilitated by mechanical stirring. The primary objective was to determine mass transfer patterns to optimize reactor design and improve energy efficiency in industrial applications. Experiments were conducted using spherical ATFB particles in a cylindrical vessel equipped with a three-blade impeller. The dissolution kinetics was examined across a temperature range of 293–323 K and impeller rotation frequencies of 1.67–6.67 s^{-1}. The results demonstrated that both temperature and rotation frequency significantly influence the rate of surface area reduction and dissolution intensity. Specifically, increasing the temperature from 293 K to 323 K resulted in a 2.58-fold increase in dissolution intensity, while increasing rotation frequency from 1.67 s^{-1} to 6.67 s^{-1} yielded a 1.9-fold increase. Analysis of the mass transfer coefficients indicated that the dissolution process operates in a diffusion-controlled regime. To generalize the experimental data, a dimensionless empirical correlation for the Sherwood number was derived: $Sh=5.8ЧRe^{0.5}ЧSc^{0.33}d_p/D_a$. The proposed model aligns with experimental results with a maximum absolute relative error of less than 6%, confirming its adequacy for engineering calculations and the prediction of ATFB dissolution rates in industrial reactors.

Keywords: ammonium tetrafluoroborate; dissolution kinetics; mass transfer intensification; mechanical stirring; Sherwood number; solid–liquid system; mass transfer coefficient.

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