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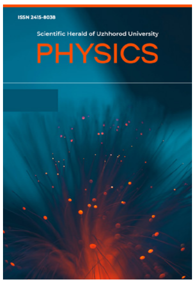

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The appearance of standing wave structures in the reaction medium during the diffusion development of the chain reaction process

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Abstract

Relevance. Understanding the dynamic behavior of radicals in reactors undergoing gas-phase oxidation of organic substances is crucial for optimizing reactor design and safety across industries.

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Purpose. This study aims to elucidate the emergence of standing wave structures influenced by feedback mechanisms in reactors with cylindrical and spherical symmetry, using mathematical principles governing the propagation of oscillations and shock waves in diffusion-driven chain reactions.

Methodology. Materials and methods for the research included a computer simulation using MATHCAD 2001i, and comparative analysis of experimental data obtained from reactor experiments. The computational modeling revealed vivid formations of standing wave structures in reactors influenced by feedback mechanisms.

Results. The impact of reverse connections in reactors with cylindrical and spherical symmetry significantly contributed to the formation of various standing wave structures of radical concentrations within the reaction zone. It was found that these structures were largely imperceptible visually and could only be observed when the reaction was accompanied by intense light emission. These visual representations served as compelling evidence of the intricate interplay between reaction kinetics and feedback effects. The study emphasized the importance of understanding and predicting the root causes of instabilities, ultimately enhancing the reliability and safety of reactors across various industries. The results demonstrated a correlation between specific feedback mechanisms and the spatial distribution of standing wave structures.

Conclusions. The derived computational patterns, as presented in this paper, provide compelling evidence supporting the feasibility of standing wave structure formation within reactors when influenced by feedback mechanisms. The study unveiled the potential for fine-tuning reactor parameters to influence the formation and stability of these structures. The findings represented a significant stride towards a more comprehensive understanding of dynamic regimes in reactors, with implications for reactor design, operation, and safety protocols. The insights garnered from uncovering standing wave structures influenced by feedback mechanisms offered valuable opportunities to optimize reactor design and operational safety, leading to more efficient and sustainable processes.

Keywords: oxidation; back bonding; modeling of dynamic modes; radicals; oscillatory phenomena; stationary process

Introduction

The study of standing wave structures within reaction mediums is of paramount relevance in chemical engineering and reactor dynamics, holding substantial implications for reactor design and safety. The inhibitory effect of formaldehyde on oxidation reactions introduces complexity, prompting an inquiry into whether inhibition alone leads to the emergence of feedback mechanisms capable of establishing oscillatory modes within the system.

Combined with recent advances in understanding the complexity of low-temperature oxidation processes in confined spaces, it has become increasingly important to combat the emergence of nonlinear relationships. Research by C. Lin *et al.* demonstrated the effects of nonlinear reaction kinetics and large inelastic strain on the oxidation process, further emphasizing the importance of understanding nonlinear relationships in oxidation reactions [1]. Moreover, recent studies of these authors shed light on how pulsation phenomena can occur as a result of the interaction of the intermediates with concentrated ionic complexes near the surface, resulting in the generation of subtle shock waves [2]. Such discoveries as T. Abrahamyan *et al.*, have profound implications not only for the operational integrity and efficiency of reactors using chain processes, but also for basic scientific research aimed at mastering these complex processes [3]. Oscillatory phenomena, including concentration and temperature fluctuations, are key issues in the field of industrial chain processes. In the context of standing wave structures, it is notable that it can lead to the development of functional gradients in which the concentration or activity of a particular component exhibits spatial variations.

This phenomenon is of particular importance in applications such as synthetic biology, where precise spatial organization is critical to the functionality of the system as wrote S. Kretschmer *et al.* [4]. Accordingly, researchers as E. Villar-Sepúlveda & A.R. Champneys are devoting themselves to studying the spatial arrangement and dynamic behavior of radicals in standing wave structures with the main goal of improving reactor design and increasing its operational safety [5]. The focus is on understanding the specific conditions and underlying mechanisms that lead to the formation of these distinctive structures. The implications of this research extend to improving reactor design and operational safety of processes involving gas-phase oxidation reactions. By revealing the spatial arrangement of radicals and the dynamic interactions, valuable information can be obtained to optimize reaction parameters, improve efficiency, and ensure safe operations. Obtaining comprehensive information and the ability to predict these phenomena is of paramount importance for reactor protection, especially in critical areas such as chemistry. In this regard, there is an urgent need for model studies focused on processes characterized by chain development as D. Gaskins *et al*. mentioned [6]. This endeavor serves a dual purpose: to anticipate and proactively develop complex processes in key sectors such as chemical engineering, energy, biology and various fields of human activity.

In light of these considerations, this study harnesses the mathematical framework governing the birth and propagation of oscillations and shock waves within diffusion-driven chain reactions. The primary aim is to delve into the establishment of standing wave structures of radicals within reactors immersed in the gas-phase oxidation of organic substances. Through this comprehensive inquiry, an effort is being made to enhance the comprehension of the dynamic behavior of radicals and spatial organization, ultimately contributing to the advancement of reactor design and operational safety.

Materials and Methods

Prior to commencing the experimental phase, an extensive review of existing literature was conducted. This involved a thorough examination of scientific publications, articles, monographs, and reports, providing a comprehensive overview of the current state of the issue surrounding the formation of structures of standing waves of radicals in reactors engaged in gas-phase oxidation of organic substances. Notably, key theoretical and experimental studies in this domain, along with the respective findings, were underscored [2; 7].

The computer modeling was executed utilizing the MATHCAD 2001i software package to validate theoretical concepts and scrutinize the behavior of the reaction medium. Within this endeavor, a mathematical model was crafted, encompassing equations elucidating the diffusion propagation of the chain reaction and the emergence of structures of standing waves of radicals. By employing MATHCAD 2001i, the numerical solution of a system of differential equations was achieved, alongside the capacity to visualize outcomes through graphs and diagrams. Following the computer modeling phase, the results thus obtained underwent a meticulous comparative analysis. This step involved a rigorous examination to ascertain the congruence or disparities between the modeled data and existing empirical evidence or theoretical predictions, thereby ensuring the robustness and accuracy of the model.

The study used mathematical modelling. The model consideration is carried out within the framework of the theory of diffusion propagation of particles with reproduction in limited volumes. The solution to the problem is reduced to solving the equation:

$$u_t = a^2 \Delta u + \beta u \text{ – inside the T area,} \tag{1}$$

where: u – concentration of active particles;$a^2 = D/c$; D – diffusion coefficient of active particles; c – porosity of the medium (in case of gas medium $c = 1$); β – reproduction rate; Δ Laplace operator.

With initial and boundary conditions:

$$u(M, 0) = \varphi(M),\ u_{\in} = 0. \tag{2}$$

As a result, a function was obtained [8]:

$$u(M, T) = \sum_{n=1}^{\infty} C_n e^{(\beta - a^2 \lambda_n)t} v_n(M), \tag{3}$$

where: C_n – number describing a curve, the contour of an arc, but in this work the behavior of the concentration of active particles depending on time and space due to periodic changes in the properties of the reaction medium is also important; λ_n – characteristic parameter which, in the case of a reactor with spherical symmetry, has the form:

$$\lambda_1 = \left(\frac{\pi}{R}\right)^2. \tag{4}$$

The use of this formula to solve the problem is more convenient, since it allows to present the complex problem of the relationship of chain oxidation processes in the most convenient way to find a qualitative picture of the influence of unnecessary connections on the type of dynamic regime in the system. Namely, the appearance of an inhibitor that destroys the leading chain radical leads to the formation of a periodic decrease and restoration of the rate of reproduction during the diffusion of active particles, by representing the coefficient β as a value periodically varying with time, namely $\beta^*|\sin(t)|$. In this approximation, equation (1) can be represented as:

$$u(M, T) = \sum_{n=1}^{\infty} C_n e^{(\beta|\sin(t)| - a^2 \lambda_n)t} v_n(M). \tag{5}$$

For simplicity, it is being considered the case of $n = 1$ and a spherically symmetric reactor. In this case, equation (2) is represented as:

$$u(M,T) = const * e^{(\beta|\sin(t)|) - D * \left(\frac{\pi}{R}\right)^2)t} * \frac{\sin\left(\frac{r}{R}\right)}{\frac{r}{R}}. \tag{6}$$

In this work, interest is focused not so much on obtaining exact numerical values characterizing the reaction, but rather on finding the range of values of these parameters leading to the establishment of standing wave structures in reactors during technological processes based on chain reactions.

Results

The investigation into the emergence of standing wave structures within the reaction medium during the progression of the diffusion-driven chain reaction process yielded compelling findings. These results provide valuable insights into the dynamic interplay of radicals and spatial organization within the reactor. To begin, it is essential to highlight the distinctive patterns and characteristics observed in the standing wave formations, shedding light on the underlying mechanisms. A quantitative analysis of key parameters, such as wave amplitude and frequency, serves to elucidate influence on the overall reaction kinetics.

The results are summarized below provide a comprehensive visual representation of the dynamic oxidation reaction of organic compounds within reactors possessing both spherical and cylindrical symmetry. This dynamic process is influenced by the presence of an inhibitory factor, either in the form of an intermediate product or through the occurrence of periodic shifts in concentration along the radical chain within the reactor wall layer.

The calculations are based on formula (2), which accommodates the introduction of an inhibitor – either an intermediate or final product of the reaction. This inhibitor exerts a significant influence on the leading chain radical, resulting in a temporary reduction in reaction rate. In cases where feedback occurs, periodic variations may manifest. This behavior is quantified by modifying the parameter β with the function $|\sin(t)|$, signifying its prevalence throughout the entire volume. Alternatively, in scenarios characterized by concentrated feedback near the reactor periphery, a factor denoted $\alpha \cdot |\sin(t)|$as is subtracted from the reactor’s diameter (in the case of spherical symmetry) or radius (in the case of cylindrical symmetry). This signifies a periodic contraction of the reactor’s dimensions, reflecting the feedback’s spatial extent. This nuanced consideration expands the understanding of the intricate interplay between reaction kinetics and inhibitor-induced dynamics.

Periodic inhibition of a process by a reaction intermediate

In the existing literature, instances have been reported where the presence of excited formaldehyde molecules, an intermediate product of the acetaldehyde oxidation reaction, disrupts the leading radical chain, resulting in the onset of an oscillatory regime in the system [7]. This phenomenon is attributed to quantum resonance, wherein the excitation energy of formaldehyde is transferred from the leading chain to the CH_3CO_3 radical, a phenomenon detailed in theoretical studies. Empirical data affirms that the introduction of formaldehyde molecules from an external source exerts an inhibitory influence on the oxidation reaction. This effect is ascribed to the conversion of highly active radicals into less reactive species. Nevertheless, it’s important to note that mere inhibition does not automatically result in the development of feedback mechanisms that can induce oscillatory dynamic modes within the system. Previous works primarily addressed scenarios involving the appearance of excited formaldehyde molecules, which were more likely to induce the formation of cold flames [2; 7]. Through simulations focusing on the generation of highly vibrationally excited formaldehyde molecules via heterogeneous recombination, a diverse range of feedback modes and intriguing phenomena were observed.

Particularly noteworthy is the proposition that feedback is concentrated near the surface, prompting inquiries into its broader impact on the overall volumetric process. This innovative perspective promises to deepen understanding of the intricate interplay between inhibition, feedback, and overall reactor dynamics. The calculation results using the MATHCAD 2001i program are shown in the Figure 1.

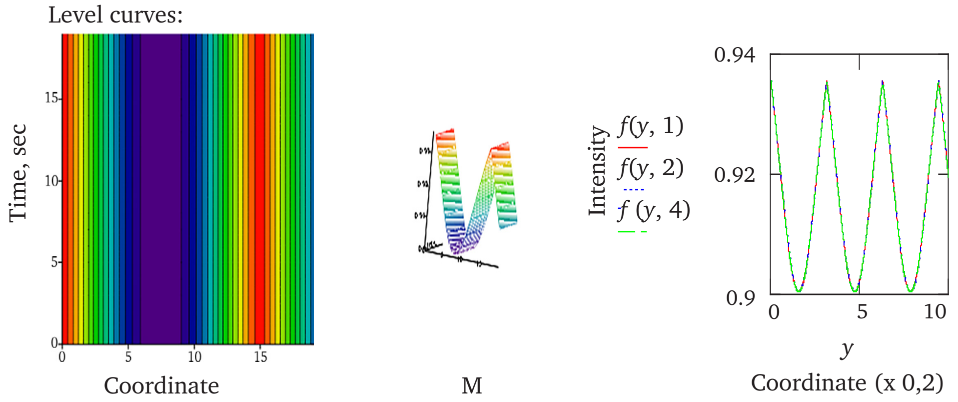

Figure 1. Establishment of the structure of standing waves in a spherical reactor due to feedback at the reactor walls calculated using the MATHCAD 2001i program
Note: according to the formula: $u(r, t) = j_s(0, \pi/(5-|\sin(t)|))$; r – coordinate; t – time
Source: developed by the authors

In the context of the stationary reaction mode, characterized by the condition $\beta - a^2\lambda_n = 0$ in equation (1), and with the radius subject to periodic variations described by $R - |\sin(t)|$, a discernible phenomenon emerges. The visual representation vividly illustrates the establishment of a standing wave structure within a reactor exhibiting spherical symmetry. This dynamic portrayal underscores the critical interplay between parameters β, α, and λ_n, demonstrating pivotal roles in shaping the distinctive patterns observed. As the reactor's radius oscillates in a periodic manner, the resulting spatial variations give rise to the formation of these intriguing standing waves [8].

While this structural phenomenon may not be readily discernible to the naked eye, it becomes detectable through sensitive sensors if the reaction is accompanied by light emission, particularly in the IR, UV, or visible spectrums. This visual insight provides a valuable perspective on the system's behavior in response to the interplay of reaction kinetics and feedback mechanisms [9]. This observation underscores the significance of specialized detection methods in revealing hidden structural intricacies within reactors. Valuable insights into the dynamic behavior of radicals and spatial organization, which are otherwise imperceptible through visual inspection alone, can be gleaned by harnessing sensitive sensors. This deeper understanding holds substantial implications for enhancing the monitoring and optimization of reactions in spherical reactors.

Periodic development of the inhibitor in the reaction medium of a spherical reactor

Figure 2 and 3 depict the outcomes of computations elucidating the impact of feedback mechanisms within the system on the reaction medium. This phenomenon leads to the emergence of a distinct standing wave structure within a reactor characterized by spherical symmetry. Notably, these visual representations showcase varying sets of characterizing parameters, providing a comprehensive view of the system's response to different conditions.

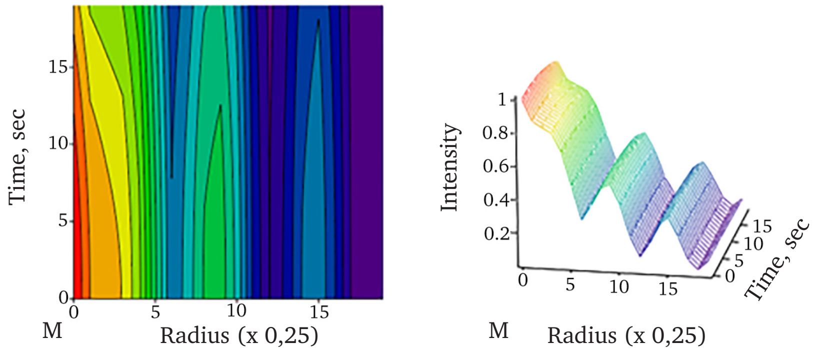

Figure 2. The structure of standing waves in the medium of a reactor with spherical symmetry in the case of the presence of nonlinear coupling in the reactor at the value of the characteristic parameters calculated using the MATHCAD 2001i program

Note: according to the formula: $u(r,t) = e^{\left(0.5*|\sin(2t)|-\frac{\pi^2}{25}\right)*t} * j_s(0,\frac{r}{5})$
Source: developed by the authors

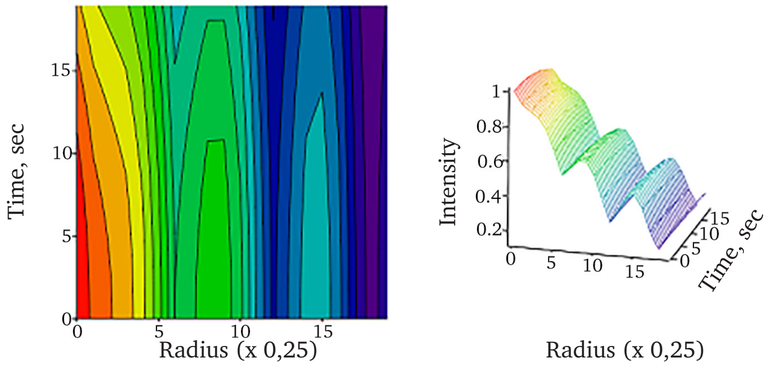

Figure 3. The structure of standing waves in the medium of a reactor with spherical symmetry in the case of the presence of nonlinear coupling in the reactor at the value of the characteristic parameters calculated using the MATHCAD 2001i program

Note: according to the formula: $u(r,t) = e^{\left(0.2*|\sin(2t)|-\frac{\pi^2}{25}\right)*t} * j_s(0,\frac{r}{5})$
Source: developed by the authors

Figures depict the formations of standing wave structures within a reactor exhibiting spherical symmetry. These structures arise in scenarios where nonlinear coupling is present, and are calculated based on the specified characteristic parameters detailed in the accompanying calculation formulas.

In these specific cases, the simulation accounts for the influence of feedback extending uniformly throughout the entire reactor volume. This dynamic process involves the periodic oscillation of the concentration of active leading radicals, with due consideration to the diffusion [10]. Consequently, this intricate interplay culminates in the establishment of a structured pattern of active radicals within the spherical reactor. These figures serve as a crucial visual testament to the sensitivity of the reaction dynamics to changes in the governing parameters. The nuanced variations in these parameters yield unique patterns and shapes in the standing wave structures, underscoring the intricate interplay between reaction kinetics and feedback effects. This comprehensive understanding further advances grasp of the system's behavior under diverse operational scenarios.

Periodic mode, concentrated near the surface of a cylindrical reactor

In the illustration below, it can be observed the distinctive structural patterns within a cylindrical reactor, specifically in the scenario where feedback manifests along the surface layer (Fig. 4). These results were obtained through computations using the MATHCAD 2001i program, utilizing specified values for the characteristic parameters. The formulation used for these calculations provides further context regarding the parameters that govern this intricate process.

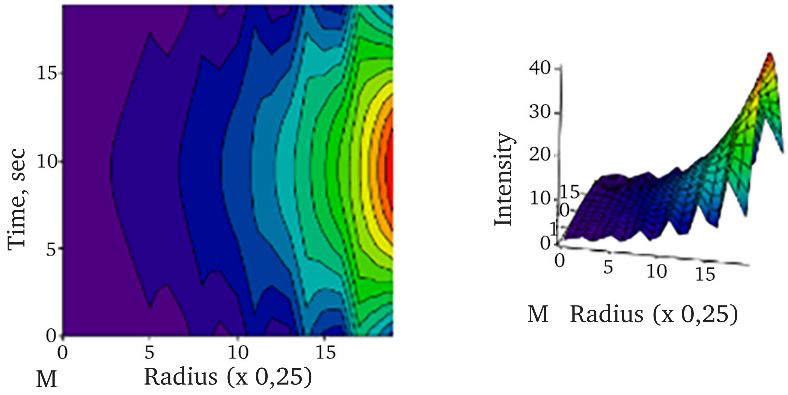

Figure 4. Formation of a structure of standing waves of concentration radicals in the case of a reactor with cylindrical symmetry at the value of the characteristic parameters calculated using the MATHCAD 2001i program

Note: according to the formula: $u(y,t) = e^{0.15*t} * 2 * J_0\left(\frac{2.4045*r}{10-4|cos(8t)|}\right)$

Source: developed by the authors

From the depicted image, it is evident that in a reactor with cylindrical symmetry, the presence of feedback leads to the establishment of a standing wave structure within the reactor volume. This observation underscores the profound impact of feedback mechanisms on the dynamic behavior of the system. Understanding the emergence of standing wave structures in reactors with cylindrical symmetry is crucial for gaining insights into the complex interplay between reaction kinetics and feedback effects. This phenomenon has significant implications for the optimization and control of processes in such reactors.

When dynamic modes are studied and the effectiveness and safety are assessed, a significant contribution can be made by recording the wave structures of radicals in the reactor if feedback occurs in the system due to the inhibition of the reaction by intermediate or final excited reaction products. In areas where the concentration of radicals is at its maximum, there is a high likelihood that the reaction radiation will be more intense. Consequently, a striped pattern can be obtained during registration allowing for the extraction of information about the nature of feedback in the reactor.

This study demonstrates the profound influence of feedback mechanisms on the spatial organization of radicals within reactors of varying symmetries. Through rigorous computational modeling and analysis, standing wave structures were observed to emerge in reactors with both spherical and cylindrical symmetry. These patterns were shown to be highly sensitive to changes in characteristic parameters, showcasing the intricate interplay between reaction kinetics and feedback effects. Additionally, the presence of nonlinear coupling in reactors with spherical symmetry further enriched the complexity of standing wave formations [11]. These findings provide valuable insights for optimizing and controlling reactions in diverse reactor configurations.

Discussion

This work introduces a novel approach, leveraging a mathematical method from existing literature to describe the propagation of chain reactions in confined volumes during the diffusion of an unstable gas. This approach provides insights into the establishment of dynamic regimes featuring standing wave structures in the system. Throughout the research, particularly noteworthy results have been obtained for the first time, shedding light on the influence of external conditions (such as heat removal, presence of excited particles, and alterations in surface properties of reaction vessels), often manifesting as feedback on systems with a chain development mechanism.

An additional point of interest lies in understanding the state of the reaction medium based on the specific structure of standing waves. By delving into this aspect, it becomes possible to anticipate the type and location of feedback within the reactor. The work of G. Sargsyan *et al*. cited elucidate the phenomenon of feedback formation near the reactor wall layer [7]. This study reveals that the presence of active centers at the vessel walls leads to the generation of excited formaldehyde molecules, which act as destructive agents for active radicals, particularly the leading chains of CH_3CO_3. This, in turn, gives rise to concentration fluctuations of these radicals in the near-surface layer of the reactor. This work, in particular, scrutinizes the impact of oscillations within the near-surface layer on the overall reactor process. The challenge is addressed by resolving the considerations of a stationary process within a reactor featuring a dynamically changing radius, specifically in cases of reactors with spherical symmetry. When the concentration of CH_3CO_3 radicals diminishes due to interactions with excited formaldehyde molecules, it is postulated that the reactor's radius contracts in proportion to the penetration depth of excited formaldehyde molecules facilitated by diffusion.

The studies outlined above provide valuable parallels and insights that complement this investigation into standing wave structures in reaction media during the diffusion-driven chain reaction process. Several key considerations for future research endeavors can be gleaned from these findings. This work aligns with the study of C.T. Hamik & O. Steinbock that explores excitation waves in reaction-diffusion media with non-monotonic dispersion relations [12]. The observations revealed the presence of rotating spiral waves and target patterns in two-dimensional excitable systems. Comparisons between results could shed light on potential commonalities and offer a basis for refining mathematical models. Another work by S. Hata *et al*. established essential conditions for wave instability in general three-component reaction-diffusion systems [13]. These conditions, expressed in terms of the Jacobian matrix of the system's uniform steady state, provide a means to determine the potential observability of wave instability with the gradual increase of species mobility. This insight can be instrumental in refining understanding of the stability and dynamics of standing wave structures, providing criteria for the emergence. In a different approach K. Regenauer-Lieb *et al*. proposed the universality of dissipative wave phenomena in Thermo-Hydro-Mechanical-Chemical (THMC) reaction-diffusion systems that operate far from equilibrium [14]. It introduced an updated formulation for chemical systems, contending that the wave operator must incorporate non-local reaction-diffusion equations. Further research could explore the applicability of this universal concept to specific context, potentially uncovering additional insights into the underlying mechanisms.

The study of D. Cuiñas *et al*. investigated the transition from traveling to standing waves in a reaction-diffusion system as a function of frequency [15]. The researchers noted that a further increase in frequency led to yet another transition, this time resulting in bulk oscillations. Future studies based on this may delve deeper into the underlying factors influencing such transitions, potentially shedding light on the nuanced interplay of feedback mechanisms in this specific system. The work of C. Hamster & P. van Heijster elucidated how stochastic patterns arising from the stochastic cell motility model equation can be harnessed to comprehend experimentally observed dynamics, particularly those pertaining to waves [16]. Understanding how stochasticity influences wave dynamics may provide valuable insights into the robustness and adaptability of standing wave structures in response to environmental perturbations. Incorporating these comparative considerations into future research endeavors holds promise for refining understanding of standing wave structures in reaction media. Additionally, it is worth noting that while the study primarily focuses on reactors with gas-phase oxidation of organic substances, the insights gained have broader implications [17]. The emergence of standing wave structures, influenced by feedback mechanisms, extends to various reaction-diffusion systems [18]. Exploring the universality of these phenomena across different contexts could open avenues for interdisciplinary research and applications in fields beyond chemical engineering.

This study highlights the importance of considering external conditions and feedback effects when designing and operating reactors. The ability to predict and control standing wave structures provides a valuable tool for optimizing process efficiency and ensuring safety [19]. This has direct relevance to industries where precise control of chemical reactions is paramount, such as in pharmaceuticals, petrochemicals, and environmental engineering. In terms of future research directions, a deeper investigation into the role of specific feedback mechanisms and interactions with different reaction pathways could yield further insights. Additionally, exploring the potential for dynamic control of standing wave structures, for example, through modulation of external conditions, presents an intriguing avenue for enhancing process flexibility and performance.

The experimental validation of the computational models and theoretical frameworks proposed in this study would be a crucial step towards real-world application. Conducting experiments to observe and quantify standing wave structures in practical reactor setups would provide empirical support for the theoretical findings. The study not only advances understanding of standing wave structures in reactors with gas-phase oxidation but also lays the groundwork for broader applications in reaction-diffusion systems [20-22]. Improved reactor design and operation, with implications for a wide range of industries, can be achieved by considering feedback mechanisms and external conditions [23; 24]. Future research avenues include exploring specific feedback mechanisms, dynamic control strategies, and experimental validation of theoretical models. investigating the potential integration of advanced computational techniques, such as machine learning algorithms, could offer a powerful tool for predicting and optimizing standing wave structures in complex reaction-diffusion systems, further enhancing the precision and efficiency of reactor operations.

Conclusions

The approach proposed in this study, specifically the use of a mathematically developed method, highlights the intricacies of establishing dynamic regimes with standing wave structures in the system. The research yielded novel and compelling insights into the impacts of external conditions, such as heat dissipation, excited particles, and changes in the surface properties of reaction vessels, often manifesting as feedback mechanisms on the dynamic behavior of chain reaction systems. A particularly noteworthy aspect explored in this work is the influence of oscillation phenomena in the near-surface layer on the overall reactor process.

The problem was addressed by considering the stationary process in a reactor with a changing radius, as in the case of a reactor with spherical symmetry. When the concentration of CH_3CO_3 radicals minimizes due to interaction with excited molecules of formaldehyde, it is assumed that the reactor radius decreases by the penetration depth of excited formaldehyde molecules due to diffusion. It becomes evident that localized feedback near the reactor walls can lead to the formation of standing wave structures within the reactor. From the presented material, it can be inferred that the registration of radical wave structures in the reactor, especially when feedback is present due to the inhibition of the reaction by intermediate or final excited reaction products, can significantly contribute to understanding dynamic regimes and assessing their efficiency and safety. Areas with maximum radical concentrations exhibited more intense reaction emissions, and therefore, the registration of such patterns can provide a striped representation.

This approach offers valuable information about the nature of feedback mechanisms in the reactor. The investigation of dynamic regimes and the evaluation of their efficiency and safety can benefit significantly from the registration of radical wave structures in the reactor. Future research directions could involve exploring different reactor geometries, varying external conditions, and expanding the understanding of the intricate interplay between feedback mechanisms and the formation of standing wave structures. This work lays the foundation for further studies in the field, providing a basis for refining reactor design and optimizing processes in chemical engineering applications.

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Conflict of Interest

None.

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Поява стоячих хвильових структур у реакційному середовищі під час дифузійного розвитку ланцюгової реакції

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Анотація

Актуальність. Розуміння динамічної поведінки радикалів у реакторах, які зазнають газофазного окислення органічних речовин, має вирішальне значення для оптимізації конструкції реактора та безпеки в промисловості.

Мета. Це дослідження має на меті з'ясувати появу структур стоячих хвиль під впливом механізмів зворотного зв'язку в реакторах із циліндричною та сферичною симетрією, використовуючи математичні принципи, що керують поширенням коливань і ударних хвиль у ланцюгових реакціях, керованих дифузією.

Методологія. Матеріали та методи дослідження включали комп'ютерне моделювання з використанням MATHCAD 2001i та порівняльний аналіз експериментальних даних, отриманих у реакторних експериментах. Розрахункове моделювання виявило яскраві утворення структур стоячої хвилі в реакторах під впливом механізмів зворотного зв'язку.

Результати. Вплив зворотних зв'язків у реакторах з циліндричною та сферичною симетрією суттєво сприяв утворенню різноманітних структур стоячої хвилі концентрацій радикалів у зоні реакції. Було виявлено, що ці структури були в основному непомітними візуально і могли спостерігатися лише тоді, коли реакція супроводжувалася інтенсивним випромінюванням світла. Ці візуальні представлення служили переконливим доказом складної взаємодії між кінетикою реакції та ефектами зворотного зв'язку. Дослідження наголошує на важливості розуміння та прогнозування основних причин нестабільності, що в кінцевому підсумку підвищує надійність і безпеку реакторів у різних галузях промисловості. Результати продемонстрували кореляцію між конкретними механізмами зворотного зв'язку та просторовим розподілом структур стоячої хвилі.

Висновки. Отримані моделі обчислень, представлені в цій статті, надають переконливі докази, що підтверджують можливість формування структури стоячої хвилі в реакторах під впливом механізмів зворотного зв’язку. Дослідження розкрило потенціал для точного налаштування параметрів реактора для впливу на формування та стабільність цих структур. Отримані результати стали значним кроком до більш повного розуміння динамічних режимів у реакторах, що має наслідки для конструкції реактора, експлуатації та протоколів безпеки. Уявлення, отримані в результаті розкриття структур стоячих хвиль, на які впливають механізми зворотного зв’язку, пропонують цінні можливості для оптимізації конструкції реактора та безпеки експлуатації, що призводить до більш ефективних і стійких процесів.

Ключові слова: окиснення; зворотний зв’язок; моделювання динамічних режимів; радикали; коливальні явища; стаціонарний процес