Modeling the kinetics of nanoparticle formation

Rebeka Szabó

PhD thesis

Supervisor: Dr. Gábor Lente

full professor

University of Pécs
Doctoral School of Chemistry
Pécs, Hungary
2024

1. Introduction

Nanoparticles ranging from a few to a few hundred nanometers play an increasingly prominent role, especially in the fields of catalysis, electronics, medicine, and environmental remediation. This is due to their small size and high surface-to-volume ratio, which endows these particles with unique properties, making them highly suitable for various applications. Although they can be obtained both naturally and synthetically, the latter is more significant, with nanoparticles primarily synthesized from noble metals, platinum metals, or transition metal oxides or sulfides.

In the context of green chemistry, the development of catalysis becomes increasingly important, as it not only accelerates the outcomes of reactions but also supports selective transformations, minimizing unnecessary by-products. Meanwhile, nanomedicine, combining nanotechnology and medical sciences, holds great promise for healthcare, playing a significant role in diagnostics (CT, MRI) and serving as drug delivery systems. However, it is essential to consider their potential toxicity and environmental impact, derived from their unique physicochemical properties.

The exceptional properties of nanoparticles mentioned above are largely influenced by their size and distribution, making it inevitable to understand the kinetics of particle formation. Among the existing models, notable ones include the Finke–Watzky model, which can be considered an advanced version of the well-established Smoluchowski model, and the LaMer model. It is also worth examining the Becker–Döring model and its extreme case known as the Lifshitz–Slyozov–Wagner model. Furthermore, the average size and distribution of nanoparticles are determined by kinetic factors and are thermodynamically unstable compared to the bulk solid phase. Therefore, controlling their size requires a careful consideration of kinetics.

2. Research objectives

The formation kinetics of nanoparticles shows similarities with polymerization processes. However, adapting existing models for a precise description of nanoparticle formation remains an ongoing challenge. It is now evident that the sizes of the particles play a crucial role in their potential applications, significantly influencing their catalytic properties and toxicity.

One of the main key goals of the research is to apply and compare various kernel functions, such as mass, surface, Brownian, and diffusion kernels, to determine the most appropriate approximation for the final nanoparticle size distribution. These kernels serve as mathematical representations of the underlying mechanisms of nanoparticle formation, allowing for a deeper understanding of the role of different kinetic factors in determining the size and its distribution of the nanoparticles.

Additionally, the thesis aims to develop a robust methodology for interpreting experimental data related to nanoparticle size distribution. By comparing advanced modeling techniques with experimental results, we can validate and refine theoretical predictions, leading to a more comprehensive understanding of the complex kinetics involved in nanoparticle formation.

3. Assumptions and methods

The model

In the generalized nucleation-growth model, the first step involves a few monomer units forming a nucleus, which then grows through a much faster, second-order reaction by adding one monomer unit to a single nanoparticle. The reaction steps and their corresponding rate equations are defined as follows:

$$\begin{aligned} &n\mathrm{M} \xrightarrow{k_\mathrm{M}} \mathrm{C}_n && n \in \mathbb{Z}^+ && \upsilon_\mathrm{M} = k_\mathrm{M}[\mathrm{M}]^n \\ &\mathrm{C}_i + \mathrm{M} \xrightarrow{K(i)k_\mathrm{g}} \mathrm{C}_{i+1} && i \geq n && \upsilon_{\mathrm{g},i} = K(i)k_\mathrm{g}[\mathrm{M}][\mathrm{C}_i] \end{aligned} \tag{1}$$

Here, the notation represents a high number of possible models. The symbols M and C_i represent the monomer unit and a nanoparticle containing exactly i monomer units, respectively. The parameter n is a positive integer, and determines the minimum number of monomer units that can form a nucleus. The constants k_M and k_g represent the rate constants for nucleation and growth, respectively, while υ_M and $\upsilon_{\mathrm{g},i}$ denote the rates of these steps. The function $K(i)$ expresses the kernel functions determining how the rate constant of nucleus growth depends on the particle size. In this work, four different kernel functions are assumed: mass kernel (directly proportional to mass or volume, $K(i) = i$), surface kernel (directly proportional to surface, $K(i) = i^{2/3}$), Brownian kernel (directly proportional to linear size, $K(i) = i^{1/3}$), and diffusion kernel (size-independent, $K(i) = 1$).

Simplifications

To simplify the mathematical treatment and reduce the number of parameters, dimensionless quantities are introduced. These quantities enable us to express the differential equations describing the concentration of nanoparticles over time in a simpler form:

$$\begin{aligned} \frac{\mathrm{d}m}{\mathrm{d}\tau} &= -n\alpha m^n - \sum_{j=n}^{\infty} K(j)mc_j \\ \frac{\mathrm{d}c_n}{\mathrm{d}\tau} &= \alpha m^n - K(n)mc_n \\ \frac{\mathrm{d}c_i}{\mathrm{d}\tau} &= K(i-1)mc_{i-1} - K(i)mc_i \qquad i > n \end{aligned} \tag{2}$$

In the equations, m represents the dimensionless concentration of monomer units, and c_i represents those of the nanoparticles. The symbol α denotes the ratio of nucleation and growth constants, while τ symbolizes the dimensionless time.

In mathematical descriptions, the use of moments is often advantageous for populations such as the one under investigation. The qth moment of nanoparticle concentrations is defined by the following equation, where q can be any real number:

$$\mu_q = \sum_{j=n}^{\infty} j^q c_j \tag{3}$$

The physical meaning of the first moment is the sum of the amount of monomer units in all of the nanoparticles. This quantity remains constant in the system according to the law of conservation of mass. The solution to the differential equation describing this is given below:

$$\mu_1 + m = 1 \tag{4}$$

The physical meaning of the zeroth moment is the concentration of nanoparticles expressed in dimensionless quantities. However, finding an analytical solution to the differential equation for this moment requires more substantial efforts, including simplification procedures.

For both the Brownian and surface kernel cases, introducing the 1/3 and 2/3 moments proves worthwhile. These moments can be estimated as the weighted geometric means of the first and the zeroth moments.

Stochastic approach

In the continuous-time, discrete-state stochastic approach, we work with molecule counts instead of concentrations, which can be considered a continuous-time Markov chain ($X(\tau) = (X_0(\tau), X_1(\tau), \ldots, X_N(\tau))$). The sum of all monomer units and the number of nanoparticles containing exactly i monomer units gives the total molecular count in our model:

$$x_0(\tau) + \sum_{i=n}^{\infty} i x_i(\tau) = N \tag{5}$$

Due to the law of mass conservation, the above equation holds at any time moment, and by counting the possible solutions (the number of solutions for a Diophantine equation), the number of states can be obtained. Solving the ordinary differential equation system describing the temporal changes in the state probabilities is challenging in this case, so our calculations are based on Monte Carlo simulations using the Gillespie algorithm. Here, the propensities for each step are defined in a manner analogous to the deterministic rate equations.

The essence of the Gillespie simulation lies in generating two independent, uniformly distributed random numbers between 0 and 1 at each step. The first random number is

used to update the time according to the following equation:

$$\tau^{\text{new}} = \tau^{\text{old}} - \frac{\ln rnd_1}{\sum_{j=1}^{N} p_j(\tau^{\text{old}})} \tag{6}$$

The second random number is used to determine which step occurs out of the possibilities with non-zero propensity. Step i happens only if the following inequality is satisfied:

$$\frac{\sum_{j=1}^{i-1} p_j(\tau^{\text{old}})}{\sum_{j=1}^{N} p_j(\tau^{\text{old}})} \leq rnd_2 < \frac{\sum_{j=1}^{i} p_j(\tau^{\text{old}})}{\sum_{j=1}^{N} p_j(\tau^{\text{old}})} \tag{7}$$

This step induces changes in the molecule counts, repeating until all propensities become zero (such a final state exists as there are no reversible steps in the scheme).

$$\begin{aligned} &x_0(\tau^{\text{new}}) = x_0(\tau^{\text{old}}) - n; x_n(\tau^{\text{new}}) = x_n(\tau^{\text{old}}) + 1, && \text{if} \quad i = 1 \\ &x_0(\tau^{\text{new}}) = x_0(\tau^{\text{old}}) - 1; x_i(\tau^{\text{new}}) = x_i(\tau^{\text{old}}) - 1; && \\ &x_{i+1}(\tau^{\text{new}}) = x_{i+1}(\tau^{\text{old}}) + 1, && \text{if} \quad i > n \end{aligned} \tag{8}$$

We conducted the simulations using codes written in Matlab for all four different kernel functions, specifying different values for n in the nucleation step. The initial molecular counts were chosen between 10^6 and 10^8 values. These, while small compared to real cases, are computationally manageable and still provide sufficiently conclusive results when compared to deterministic calculations. The ratio of rate constants, i.e., α, was always chosen to be much smaller than 1, as the growth step needs to be much faster to reach meaningful particle sizes.

4. Results

In order to determine the dimensionless total concentration of nanoparticles, the analytical solutions for the zeroth moment need to be found for different kernel functions. As a first approximation, we consider the dimensionless concentration of monomer units as a function of μ_0:

$$\frac{\mathrm{d}m}{\mathrm{d}\mu_0} \cong -\frac{m\sum_{j=n}^{\infty} K(j)c_j}{\alpha m^n} \tag{9}$$

The solutions obtained using the approximate method for the final size of nanoparticles, as well as their non-scaled forms, are summarized in Table 1.

Table 1: Final size of nanoparticles for different kernel functions

Kernel functions	**Average final particle size** ($\bar{M}_\infty$)
Diffusion kernel	$\sqrt{\frac{nk_\mathrm{g}}{2[\mathrm{M}]_0^{n-2}k_\mathrm{M}}}$
Surface kernel	$\sqrt[4]{\frac{27}{64}}\left(\frac{[\mathrm{M}]_0^{n-2}k_\mathrm{M}}{nk_\mathrm{g}}\prod_{j=1}^{n}\frac{3j}{3j-2}\right)^{-3/4}$
Brownian kernel	$\left(\frac{3}{5}\right)^{3/5}\left(\frac{[\mathrm{M}]_0^{n-2}k_\mathrm{M}}{nk_\mathrm{g}}\prod_{j=1}^{n}\frac{3j}{3j-1}\right)^{-3/5}$
Mass kernel ($n=1$)	$\frac{[\mathrm{M}]_0 k_\mathrm{g}}{\ln\left(1+\frac{[\mathrm{M}]_0 k_\mathrm{g}}{k_\mathrm{M}}\right)k_\mathrm{M}}$
Mass kernel ($n>1$)	$\frac{[\mathrm{M}]_0^{-n}\left([\mathrm{M}]_0^2+[\mathrm{M}]_0^n nk_\mathrm{M}\right)\left(1+\frac{[\mathrm{M}]_0^{n-2}nk_\mathrm{M}}{k_\mathrm{g}}\right)^{-n}}{\ln\left(1+\frac{[\mathrm{M}]_0^{2-n}k_\mathrm{g}}{nk_\mathrm{M}}\right)k_\mathrm{M}}\sum_{i=1}^{n-1}\frac{1}{i}\frac{[\mathrm{M}]_0^{2-n}k_\mathrm{g}\left(1+\frac{[\mathrm{M}]_0^{n-2}k_\mathrm{M}}{k_\mathrm{g}}\right)^{1+i-n}}{k_\mathrm{M}}$

To validate the accuracy of our calculations, we compared them with the results of precise stochastic simulations, as shown in Figure 1 for five different cases of the Brownian kernel ($n = 1, 2, 3, 4, 5$).

For the temporal evolution of nanoparticle concentrations, exact analytical solutions could be found in only three cases. The first is the case of the diffusion kernel with first-order nucleation ($n = 1$):

$$[\mathrm{C}_i] = -\frac{1}{[\mathrm{M}]_0 k_\mathrm{g}}\left(e^{\frac{k_\mathrm{M}\left(k_\mathrm{M}-[\mathrm{M}]_0 k_\mathrm{g}\sqrt{\frac{k_\mathrm{M}(2[\mathrm{M}]_0 k_\mathrm{g}+k_\mathrm{M})}{[\mathrm{M}]_0^2 k_\mathrm{g}^2}}\right)\tanh\left(\mathrm{ArcTanh}\left[\sqrt{\frac{k_\mathrm{M}}{2[\mathrm{M}]_0 k_\mathrm{g}+k_\mathrm{M}}}\right]+\frac{1}{2}[\mathrm{M}]_0 t k_\mathrm{g}\sqrt{\frac{k_\mathrm{M}(2[\mathrm{M}]_0 k_\mathrm{g}+k_\mathrm{M})}{[\mathrm{M}]_0^2 k_\mathrm{g}^2}}\right)}{[\mathrm{M}]_0^2 k_\mathrm{g}^2}} - 1\right) \tag{10}$$

$$k_\mathrm{M}\sum_{j=0}^{i-1}\frac{1}{j!}\left(\frac{[\mathrm{M}]_0 k_\mathrm{g}\sqrt{\frac{k_\mathrm{M}(2[\mathrm{M}]_0 k_\mathrm{g}+k_\mathrm{M})}{[\mathrm{M}]_0^2 k_\mathrm{g}^2}}\tanh\left(\frac{1}{2}[\mathrm{M}]_0 t k_\mathrm{g}\sqrt{\frac{k_\mathrm{M}(2[\mathrm{M}]_0 k_\mathrm{g}+k_\mathrm{M})}{[\mathrm{M}]_0^2 k_\mathrm{g}^2}}+\tanh^{-1}\left(\sqrt{\frac{k_\mathrm{M}}{2[\mathrm{M}]_0 k_\mathrm{g}+k_\mathrm{M}}}\right)\right)}{k_\mathrm{M}} - 1\right)$$

Symbolic solutions were also successfully found for the mass kernel when nucleation is

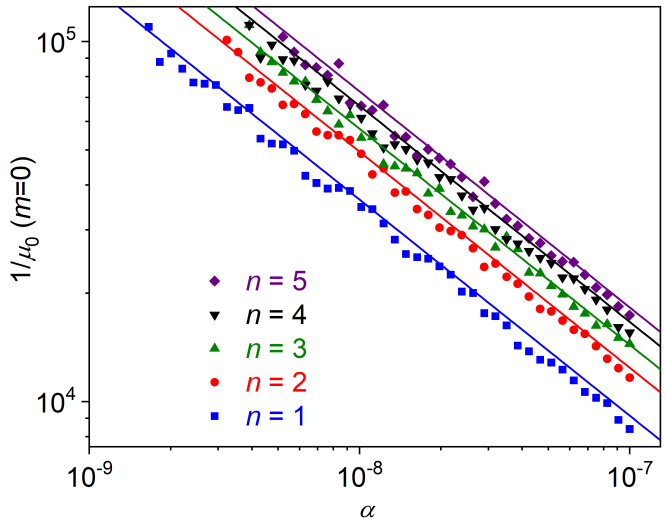

Figure 1: Average final nanoparticle size as a function of the ratio of the nucleation and growth rate constants for the Brownian kernel with $n = 1, 2, 3, 4, 5$. The markers represent the results of stochastic simulations, while the lines depict the deterministic formulas.

first- ($n = 1$) and second-order ($n = 2$):

$$[\mathrm{C}_i] = \frac{\left(1 - e^{-\frac{t([\mathrm{M}]_0 k_\mathrm{g} + k_\mathrm{M})}{[\mathrm{M}]_0^2}}\right) k_\mathrm{M}}{i\left([\mathrm{M}]_0 k_\mathrm{g} + k_\mathrm{M}\right)} \tag{11a}$$

$$\begin{aligned}[\mathrm{C}_i] = {} & \frac{[\mathrm{M}]_0 2 k_\mathrm{g}^{i-2} k_\mathrm{M}^2 (i-1)}{(2k_\mathrm{M} + (k_\mathrm{g} - 2k_\mathrm{M}) e^{-[\mathrm{M}]_0 k_\mathrm{g} t})} \prod_{j=2}^{i} (2k_\mathrm{M} - k_\mathrm{g} j - k_\mathrm{g}) \\ & + [\mathrm{M}]_0 \sum_{j=2}^{i} \frac{k_\mathrm{M}\left(j^2 - 1\right)}{\left(2k_\mathrm{M} - k_\mathrm{g} j - k_\mathrm{g}\right) j} \binom{i-1}{j-1} (-1)^j \\ & \left[\left(\frac{k_\mathrm{g}}{2k_\mathrm{M} + (k_\mathrm{g} - 2k_\mathrm{M}) e^{-[\mathrm{M}]_0 k_\mathrm{g} t}} \right)^{\frac{k_\mathrm{g}}{2k_\mathrm{M} - k_\mathrm{g}}} - 1 \right]\end{aligned} \tag{11b}$$

In all other cases, numerical calculations are required to determine the time-dependent c_i variables.

5. Thesis points

1. **A family of generalized nucleation-growth models for the kinetic description of nanoparticle formation has been introduced, in which the size-dependent reactivity of individual nanoparticles is represented by a kernel function**. In the first step, a few monomer units (n) form a nucleus, which then grows further in second-order steps by attaching other single monomer units consecutively. We assumed four types of kernel functions: mass, surface, Brownian, and diffusion kernels. The system of differential equations describing the temporal change in concentrations was provided with dimensionless quantities and, for simplicity in mathematical treatment, the moments were also applied.

2. **General symbolic solutions for the temporal evolution of concentrations were found for the diffusion kernel** ($n = 1$) **and two cases of the mass kernel** ($n = 1, 2$)**.** For all other cases, numerical computations and often also approximations are necessary.

3. **An appropriate approximate differential equation for the zeroth moment (total nanoparticle concentration) has been introduced.** We obtained symbolic solutions for the average final nanoparticle size for all four kernel functions, regardless of the value of n.

4. **The developed approximations have been validated against Gillespie simulations.** We carried out exact stochastic simulations for all the kernel functions with all possible values of n employing the Gillespie algorithm. A code in Matlab was written to implement the method. The error caused by the approximations were characterized by comparison with the exact stochastic simulations and were found to be practically negligible.

Publications

Publications related to the thesis

1. **Szabó, R.,** Lente, G. Full analytical solution of a nucleation-growth type kinetic model of nanoparticle formation, *J. Math. Chem.*, **2019**, 57, 616-631. **IF: 1.77**

2. **Szabó, R.,** Lente, G. A comparison of the stochastic and deterministic approaches in a nucleation-growth type model of nanoparticle formation, *Chem. Mat.*, **2021**, 33, 5430-5436. **IF: 10.51**

3. **Szabó, R.,** Lente, G. General nucleation-growth type kinetic models of nanoparticle formation: possibilities of finding analytical solutions, *J. Math. Chem.*, **2021**, 59, 1808-1821. **IF: 2.48**

4. **Szabó, R.,** Lente, G. Predicting particle size distribution in nanoparticle formation by stochastic and deterministic approaches, *Željko Čupić; Slobodan Anič (ed.), PHYSICAL CHEMISTRY 2021. (Proceedings)*, **2021**, pp. 123-128.

5. Lente, G., **Szabó, R.,** Matematikai reakciókinetika: a paritássértési energiától a nanorészecske-növekedésig, *Magy. Kém. Foly.*, **2022**, 128, 60-68.

6. **Szabó, R.,** Lente, G. Deterministic approximation for the nucleation-growth type model of nanoparticle formation: a validation against stochastic simulations, *Chem. Eng. J.*, **2022**, 445, 137377. **IF: 15.1**

Posters and presentations related to the thesis

1. Lente, G., **Szabó, R.** Detailed kinetic analysis of a simple two-step nanoparticle growth model, 1st International Conference on Reaction Kinetics, Mechanism and Catalysis, June 6-9, 2018, Budapest, Hungary

2. **Szabó, R.,** Lente, G. Analytical solution of a nucleation-growth type model of nanoparticle formation, Joint Meeting of the Coordination Chemistry Working Group and the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, November 8-9, 2018, Veszprém, Hungary

3. **Szabó, R.,** Lente, G. A comparison of the stochastic and deterministic approach in a nucleation-growth type model of nanoparticle formation, 3rd Workshop on Formal Reaction Kinetics and Related Areas, Budapest University of Technology and Economics, January 9-10, 2020, Budapest, Hungary

4. **Szabó, R.,** Lente, G. Comparison of the stochastic and deterministic approach in a nucleation-growth type model of nanoparticle formation, Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences (online), November 6, 2020

5. **Szabó, R.,** Lente, G. Comparison of the stochastic and deterministic approach in a nucleation-growth type model of nanoparticle formation, 9^{th} Interdisciplinary Doctoral Conference (online), November 27-28, 2020

6. **Szabó, R.,** Lente, G. Symbolic deterministic and simulation stochastic description of nanoparticle formation kinetics, Formal Reaction Kinetics Seminar (online), February 25, 2021

7. **Szabó, R.,** Lente, G. A comparison of the stochastic and deterministic approach in a nucleation-growth type model of nanoparticle formation, 2^{nd} International Conference on Reaction Kinetics, Mechanism and Catalysis (online), May 20-22, 2021

8. **Szabó, R.,** Lente, G. Symbolic deterministic and simulation stochastic description of nanoparticle formation kinetics, II. FKF Szimpózium (online), June 16-18, 2021

9. Lente, G., **Szabó, R.** Predicting particle size distribution in nanoparticle formation by stochastic and deterministic approaches, PHYSICAL CHEMISTRY 2021. 15^{th} International Conference on Fundamental and Applied Aspects of Physical Chemistry, September 20-24, 2021, Belgrade, Serbia

10. **Szabó, R.,** Lente, G. A comparison of the stochastic and deterministic approach in a nucleation-growth type model of nanoparticle formation, Mathematics in (bio)Chemical Kinetics and Engineering 2021 (online), October 24-27, 2021, Shanghai, China

11. **Szabó, R.,** Lente, G. A comparison of the stochastic and deterministic approach in a nucleation-growth type model of nanoparticle formation, 10^{th} Jubilee Interdisciplinary Doctoral Conference, November 12-13, 2021, Pécs, Hungary

12. **Szabó, R.,** Lente, G. Deterministic approximation for the nucleation-growth type model of nanoparticle formation: comparison with stochastic results, Formal Reaction Kinetics Seminar (online), February 22, 2022

13. **Szabó, R.,** Lente, G. Deterministic approximation for the nucleation-growth type model of nanoparticle formation: comparison with stochastic results, Intelligens szakosodás megvalósítása a Pécsi Tudományegyetemen (online), March 21-23, 2022

14. **Szabó, R.,** Lente, G. Deterministic approximation for the nucleation-growth type model of nanoparticle formation: comparison with stochastic results, 20^{th} János Szentágothai Conference and Competition (online), April 14, 2022

15. **Szabó, R.,** Lente, G. Deterministic approximation for the nucleation-growth type model of nanoparticle formation: comparison with stochastic results, Spring Wind Conference, May 6-8, 2022, Pécs, Hungary

16. **Szabó, R.,** Lente, G. Deterministic approximation for the nucleation-growth type model of nanoparticle formation: comparison with stochastic results, Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, May 19-20, 2022, Balatonvilágos, Hungary

17. **Szabó, R.,** Lente, G. Prediction of nanoparticle size distributions based on nucleation-growth type models, ACS Fall 2022, Chicago, Il, USA

18. Lente, G., **Szabó, R.** Nucleation-growth type models of nanoparticle formation: deterministic and stochastic approaches, Workshop on Aerogels Characterization and Modelling, March 29-31, 2023, Debrecen, Hungary

19. **Szabó, R.,** Lente, G. Prediction of nanoparticle size distributions based on nucleation-growth type models, 21^{st} János Szentágothai Conference and Competition (online), April 21, 2023

20. Lente, G., **Szabó, R.** Kinetic description of nanoparticle formation, Joint Meeting of the Surface Chemistry and Nanoscale Structure Working Group, Catalysis Working Group and Colloid Chemistry Working Group of the Hungarian Academy of Sciences, May 24, 2023, Budapest, Hungary

21. **Szabó, R.,** Lente, G. Modeling the kinetics of nanoparticle formation, ACS Fall 2023, August 13-17, 2023, San Francisco, Ca, USA

22. **Szabó, R.,** Lente, G., Bibbona, E., Cappelletti, D., Siri, P., Sabbioni, E. Mathematical kinetic analysis of nanoparticle formation models, Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, October 26-27, 2023, Mátrafüred, Hungary

23. **Szabó, R.,** Lente, G., Bibbona, E., Cappelletti, D., Siri, P., Sabbioni, E. Final nanoparticle size distribution under unusual parameter regimes, Formal Reaction Kinetics and Related Questions Seminar (online), October 31, 2023

Publications not related to the thesis

1. Lente, G., Fursenko, A., **Szabó, R.** Use of the Taylor theorem to predict kinetic curves in an arbitrary mechanism, *Chem. Eng. J.*, **2022**, 445, 136676. **IF: 15.1**

2. Kumar, S. K. A., Lente, G., Szabó, R. A polynomial-based method to approximate kinetic curves in multistep mechanism, *Željko Čupić; Slobodan Anič (ed.), PHYSICAL CHEMISTRY 2022. (Proceedings)*, **2022**, pp. 127-134.

3. Lente, G., **Szabó, R.** Hidrogéntechnológiai kutatások a Megújoló Energiák Nemzeti Labor első évében, *Magy. Kém. Foly.*, **2023**, 129, 87-88.

4. Sabbioni, E., **Szabó, R.**, Siri, P., Cappelletti, D., Lente, G., Bibbona, E. Final nanoparticle size distribution under unusual parameter regimes, *submitted*, preprint at ChemRxiv, **2024**, doi:10.26434/chemrxiv-2024-wh3jv.

Popular science article

1. Lente, G., **Szabó, R.** Gyalogos tudomány az Alpok árnyékában, *Magy. Kém. Lapja*, **2024**, 79(1), 12-14.

Posters and presentations not related to the thesis

1. Lente, G., **Szabó, R.** Chiral symmetry breaking in crystallization equilibrium, Mathematics in (bio)Chemical Kinetics and Engineering 2017, May 25-27, 2017, Budapest, Hungary

2. **Szabó, R.,** Lente, G. Chiral symmetry breaking in crystallization equilibrium, Meeting of the Reaction Kinetics and Photochemistry Working Group of the Hungarian Academy of Sciences, November 2-3, 2017, Budapest, Hungary

3. Lente, G., Fursenko, A., **Szabó, R.** Use of the Taylor theorem to predict kinetic curves in an arbitrary mechanism, Mathematics in (bio)Chemical Kinetics and Engineering 2021 (online), October 24-27, 2021, Shanghai, China

4. Kumar, A.K.S., Lente, G., **Szabó, R.** A polynomial-based method to approximate kinetic curves in multistep mechanism, PHYSICAL CHEMISTRY 2022. 16^{th} International Conference on Fundamental and Applied Aspects of Physical Chemistry, September 26-30, 2022, Belgrade, Serbia