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A cellular automata framework to study the diffusion in single and binary solvent systems

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In this work, we present a two-dimensional cellular automata (CA) model to study mass transfer by diffusion of molecules in single and binary solvent systems. The method builds on Vanag's probabilistic cellular automata (PCA), where diffusion is simulated through stochastic exchange of molecules between neighboring cells. While the original PCA framework effectively models single component diffusion driven by concentration gradients, it could not account for variable diffusion coefficients. We address this limitation by generalizing the PCA approach to handle binary systems, enabling the simulation of diffusion in heterogeneous materials with varied transport properties. This extension broadens the applicability of CA-based methods for capturing complex diffusion dynamics.

Keywords Diffusion, Mass transfer, Single component, Binary components, Cellular automata, Lattice model

Mass transfer plays a crucial role in the separation processes such as extraction, distillation and absorption. These processes involve the transfer of mass between two or more phases and are used to separate mixtures into their component parts¹. Diffusion is the primary mechanism driving mass transfer at the molecular level¹.

Understanding diffusion in complex media such as gels and membranes is essential due to the heterogeneous and multiscale nature of these systems. This significantly influences the transport properties and, consequently, the efficiency of separation processes. In biological membranes, diffusion occurs primarily via small molecules crossing lipid bilayers. The interaction of molecules with the membrane matrix and the dynamic structural organization of lipids create selective permeability and influence diffusion rates².

In hydrogels, widely studied for their applications in controlled release^{3,4} and filtration⁵, the diffusion properties can vary broadly depending on the polymer matrix composition, cross-linking density, and the presence of pores or channels within the gel structure^{6,7}.

The effects of microstructure, chemistry, and molecular motion in these complex media make diffusion a widely explored area. Advanced modeling approaches such as kinetic Monte Carlo methods⁸, and neural network-based simulations⁹, have emerged to reveal mechanistic insights and guide the design of materials and processes with tailored diffusion properties.

Cellular automata (CA) are a powerful computational modeling framework that discretizes space and time into cells with defined states evolving according to local rules. Originally proposed by John von Neumann¹⁰, CA are capable of simulating complex spatiotemporal phenomena by the interaction of cells with their neighbors, making them suitable to model a variety of physical processes including diffusion¹¹, crystallization¹², and chemical reactions¹³.

The works of Kier et al.¹⁴, and Chopard and Droz¹⁵ in the early 1990s mark a foundational advancement in the use of CA for simulating diffusion in complex systems. Kier et al.¹⁴ extended dynamic CA simulations to model water and aqueous solutions. The approach was validated by reproducing real diffusion behaviors dependent on temperature and solute lipophilicity, and exploring solute interactions that alter diffusion paths and rates as they offer insights into biological and chemical environments where multiple species coexist. In parallel, Chopard and Droz¹⁵ developed a probabilistic CA algorithm capable of efficiently simulating the random walk of many particles, showing that key physical principles are preserved, while macroscopic transport follows the telegraphist's equation and allows for the adjustment of diffusion constants and reaction terms. Their model

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delivers both computational efficiency and exact theoretical analysis, enabling systematic control of simulation scales and providing interpretations for finite-size and multiscale effects in diffusion.

Building on these foundations, the work of Weimar¹⁶ introduced a systematic construction of cellular automata algorithms for simulating reaction–diffusion systems. By using a moving average technique for diffusive dynamics and a probabilistic table lookup for reactive steps, Weimar's approach achieved quantitative agreement with analytical solutions and standard numerical techniques, while enabling strong discretization well-suited for the CA paradigm. The efficiency of this simulation approach is particularly notable for handling complex, nonlinear reactive terms. As a massively parallel model, Weimar's cellular automata could be efficiently implemented on distributed computing platforms with adaptive load-balancing, making large-scale reaction–diffusion studies feasible.

In the work of Gurikov et al.¹⁷, the transport phenomena in porous media based on the 2D Margolus partitioning cellular automaton¹⁸ are introduced. The Margolus CA model¹⁹ features synchronous computation allowing efficient parallelism where an ideal gas molecular diffusion is described. The authors extend this by incorporating thermodynamic factors such as free energy and local equilibrium which enable modeling of diffusion, adsorption, directed flow, and chemical reactions. More broadly, block-partitioned CA of this type have been shown to reproduce non-trivial transport phenomena beyond the reach of simpler continuum theories. Pintus et al.²⁰ demonstrated that a Margolus-partitioned block CA reproduces the CO₂-driven segregation effect in binary zeolite diffusion, a behavior that Maxwell–Stefan theory fails to capture even qualitatively, while Bandman²¹ provides a formal analysis of the trade-off between stochasticity and parallelization efficiency in block-synchronous CA, offering a principled basis for the block-partitioning strategy adopted in such models. The diffusion process can be effectively captured by CA through rules defining local mass transfer between neighboring cells. This local interaction approach allows CA models to represent the dynamics of diffusion beyond conventional continuous models, particularly in heterogeneous or irregular environments, where the transport domain may be structurally complex or evolving, a regime that is comparatively difficult for finite-difference, finite-element, or fixed-lattice kinetic Monte Carlo methods to address without explicit remeshing or geometry tracking.

More recently, CA-based approaches have been reviewed by Menshutina et al.²². This review catalogs CA applications across a broad range of problems in chemistry and chemical engineering spanning diffusion, crystallization, corrosion, adsorption and chemical reaction modeling. The authors highlight the recurring advantages of the approach, such as modularity (submodels for diffusion, reaction and phase change can be combined), the ability to bridge micro-, meso- and macroscale phenomena without resolving every molecular degree of freedom, and straightforward parallelization. Recently, Ding et al.²³ used a two-dimensional CA to model copper corrosion by gallium-based liquid metals, where gallium atoms diffuse and react with copper to form different intermetallic layers depending on a local concentration gradient. The model reproduced experimental layer thicknesses and the expected parabolic growth law, showing how a locally computed gradient can govern transformation outcomes. A related principle underlies the work of Robben²⁴, who built a 3D CA on the sodalite cage network in which cage-template reaction outcomes are likewise governed by local neighborhood conditions, reproducing experimental domain sizes and reaction kinetics for two cage-template reactions.

In our work, we develop a two-dimensional probabilistic CA (PCA) to model diffusion of molecules in single and binary component systems. We employ Vanag's probabilistic cellular automata²⁵, which simulates molecular diffusion by exchanging molecules between neighboring cells based on defined probabilities and complete mixing assumptions within the set of selected cells. The model uses a random number generator to determine molecule distribution after diffusion between adjacent cells which effectively captures single component diffusion due to concentration gradients. However, PCA's original framework could not handle systems with variable diffusion coefficients. To address this in our work, we extend Vanag's PCA framework for binary systems, which is useful for the simulation of diffusion in complex systems. This enhancement overcomes earlier limitations by incorporating probabilities, which account for the variable diffusion coefficients by expanding the applicability of cellular automata methods for modeling diffusion in heterogeneous materials. With further enhancements, the developed framework allows the incorporation of treatment of polymer fibers, which can be extended to polymer gels, as shown in Fig. 1, which is explored in our companion study²⁶. Fig. 1 shows the hierarchical transition from the physical gel structure to its translation into the modeling framework. It shows how diffusive environments in polymeric materials are reduced to interacting lattice sites in cellular automata that allow the simulation of molecular diffusion within the gel structure.

Development of computational methods

Single component diffusion

In this study, diffusion was modeled as the stochastic exchange of molecules between von Neumann neighbor cells (excluding diagonals) on a discrete two-dimensional lattice framework. A diffusion block was implemented using Margolus partitioning scheme, where the lattice was alternately divided into odd and even blocks. Within each block, one cell was selected at random, and a second cell was chosen from its orthogonal neighbors. The diffusion between these two cells was executed. Molecules were then redistributed based on predefined probabilities: equal distribution was the most likely outcome and highly uneven distributions were assigned lower probabilities, as shown in Eq. 1. Once all blocks were updated, one full iteration of the simulation was completed. This represents one time step. In our model, diffusion proceeded synchronously until the total number of time steps was reached, unlike Vanag's approach²⁵, where the model operated asynchronously.

$$W(m, k \mid r, s) = \frac{(r+s)!}{k!m!} \theta^k (1-\theta)^m \quad (1)$$

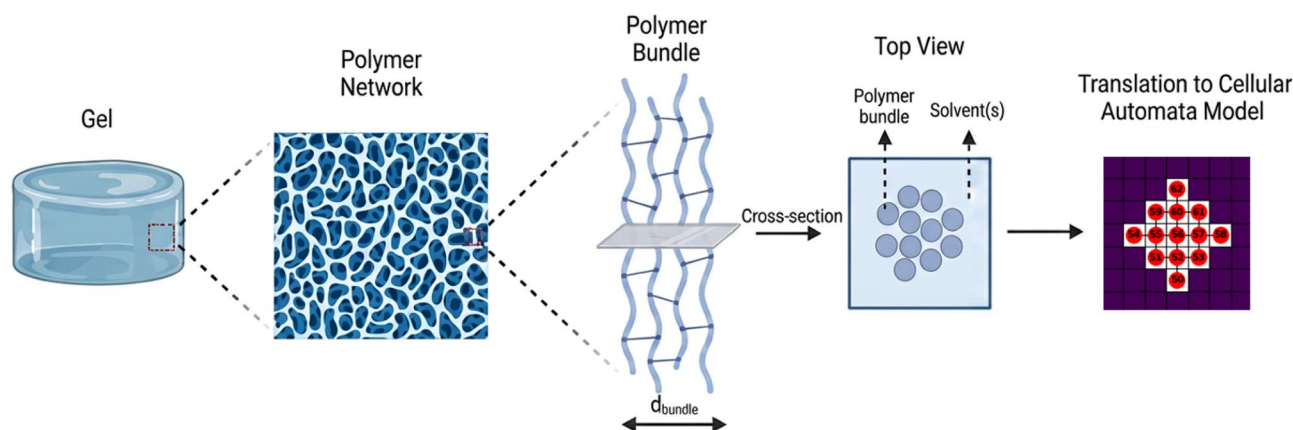


Fig. 1. Scheme showing the representation of polymer bundle in solvent in cellular automata model.

Eq. 1 from Vanag²⁷ calculates the distribution of molecules r and s before the diffusion to m and k after the diffusion event has happened. Here, θ is the ratio of volume of the lattice cell to the volume of the coalesced cells, which is 0.5 in our case. To further validate the model for molecular diffusion, non-steady-state diffusion scenarios were examined by calculating the diffusion coefficients (D) at different time steps. Two cases were considered:

- Case 1 - Instantaneous line source:

A height (H) x length (L) lattice was initialized with an amount A deposited along the lattice column $x = \frac{L}{2}$, as shown in Fig. 2a. Each cell along this line contained 25 molecules, with a maximum cell occupancy of 30 molecules, assuming a lattice cell length of 1 nm, corresponding to a cell volume of 1 nm³. This maximum cell occupancy was chosen to match the molecular number density of liquid water at ambient conditions, as shown in Eq. 2. Diffusion was simulated for 250 iterations. To obtain the average and the standard deviation for the concentration profiles $C(x, t)$ and corresponding diffusion coefficient D at time t , the diffusion process was repeated 100 times.

$$n = \frac{\rho N_A}{M} = \frac{(1000 \text{ kg m}^{-3})(6.022 \times 10^{23} \text{ mol}^{-1})}{0.018 \text{ kg mol}^{-1}} \approx 33.4 \text{ nm}^{-3} \quad (2)$$

Here, n is the molecular number density, ρ is the density of liquid water, N_A is Avogadro's constant, and M is the molar mass of water. The values of D were obtained by fitting normalized concentration profiles (C/A) against the analytical solution from Eq. 3. The concentration $C(x)/A$ was obtained from the average number of molecules present in the column x over the total number of molecules that could be accommodated in column x .

$$C(x, t) = \frac{A}{2\sqrt{\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \quad (3)$$

Eq. 3, given by Crank²⁸, represents the theoretical concentration front for the instantaneous line source.

- Case 2 - Instantaneous point source:

An $H \times L$ lattice was prepared with all molecules placed in the central cell at $t = 0$, as shown in Fig. 3a. A maximum occupancy of 1,005 molecules was considered. Diffusion was simulated for 250 iterations and the process was repeated 100 times to obtain the radial concentration profiles up to radius using Euclidean distance formula as shown in Eq. 4:

$$r = \sqrt{(x_1 - o_1)^2 + (x_2 - o_2)^2} \quad (4)$$

Here, x_1, x_2 , are the row and column indices of a given lattice cell and o_1, o_2 , are the row and column indices of the origin lattice cell. The analytical solution employed for validation, obtained from Crank²⁸ that represents the theoretical concentration front for the instantaneous point source is:

$$C(r, t) = \frac{A}{4\pi Dt} \exp\left(-\frac{r^2}{4Dt}\right) \quad (5)$$

To evaluate the constraints on local concentrations, different treatments for exceeding the maximum cell occupancy were tested, which are as follows:

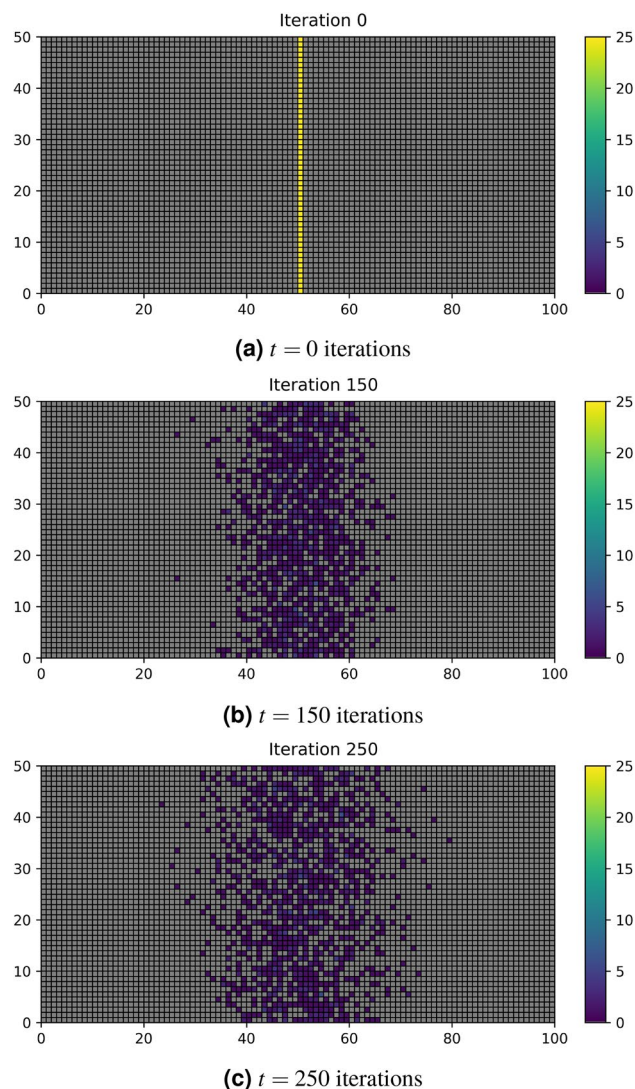


Fig. 2. Diffusion of single component on an infinite plane sheet of dimensions $H = 50$, $L = 100$, from an instantaneous line source at the center $x = \frac{L}{2} = 50$, where x ranges from 0 to 100. The set of yellow cells represents the central column with each cell containing 25 molecules. The color scale denotes the number of molecules in the cells. The images represent the snapshots from one simulation.

- rejecting the iteration,
- permitting unlimited occupancy,
- enforcing equal distribution, and
- transferring excess molecules to a neighboring cell.

All approaches produced similar deviations in D , which was fitted to the corresponding analytical solution, and the first restrictive condition was adopted for consistency in subsequent modeling.

Binary component diffusion

Binary diffusion was modeled by extending the cellular automata framework to account for concentration-dependent transport. In this approach, each lattice cell could contain a maximum (N_{max}) of 30 molecules. The number stored in a cell represented molecules of substance 1, while the remainder up to 30 corresponded to molecules of substance 2. This formulation ensured that each site was always fully populated, thereby avoiding empty or vacuum states. In this version of the model, the differences in molecular sizes between different molecules were not accounted for.

The original probabilistic cellular automata (PCA) model by Vanag assumes constant diffusion coefficients. To generalize it for binary systems such as ethanol-water mixtures, we introduced a concentration-dependent probability of diffusion, $p(C_1)$, where C_1 denotes the mole fraction of substance 1. A diffusion event occurs between cells a and b if $p(C_1) > \epsilon$, with $\epsilon \in (0, 1)$ being a uniformly distributed random number. Three strategies were tested:

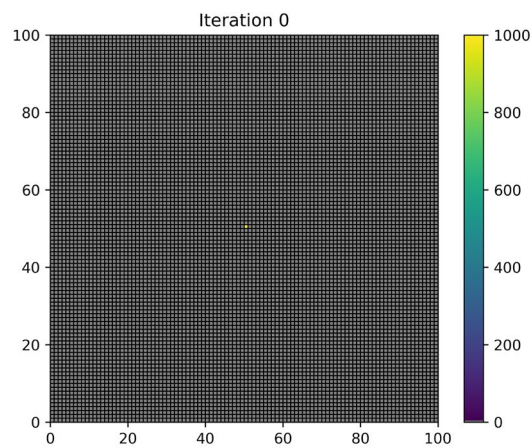
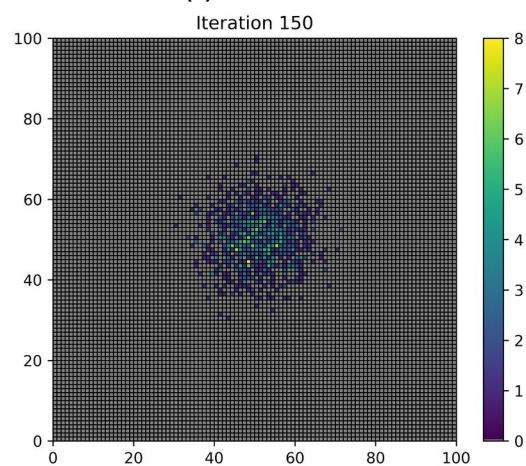
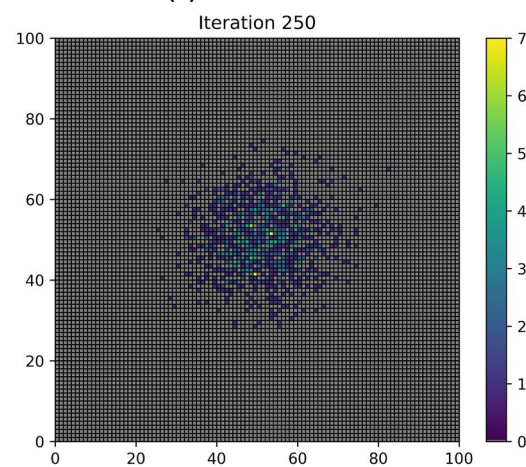
(a) $t = 0$ iteration(b) $t = 150$ iterations(c) $t = 250$ iterations

Fig. 3. Diffusion of single component on an infinite plane sheet of dimensions $H = 100$, $L = 100$, from an instantaneous point source at the center, where $r = 50$. The yellow cell represents the central cell with 1,000 molecules. The color scale denotes the number of molecules in the cells. The images represent the snapshots from one simulation.

- Case 1:

$$\bar{C}_1 = \frac{n_1^{(a)} + n_1^{(b)}}{2N_{\max}} \quad \text{and} \quad p(\bar{C}_1) > \epsilon \quad (6)$$

- Case 2:

$$\max\{p(C_1^{(a)}), p(C_1^{(b)})\} > \epsilon \quad (7)$$

- Case 3:

$$p(C_1^{(a)} \text{ or } C_1^{(b)}) = p(C_1^{(a)}) + p(C_1^{(b)}) - p(C_1^{(a)})p(C_1^{(b)}) > \epsilon \quad (8)$$

These three strategies were implemented to assess different hypotheses of how local composition might drive diffusion: averaging concentrations across two regions (Case 1), emphasizing stronger local conditions (Case 2), or accounting for the combined effect of both cells (Case 3).

If the probability condition was not satisfied, the event was skipped and the algorithm proceeded to the next block. If the event was skipped, this corresponded to a locally slower diffusion rate. However, since the probability was recalculated and checked against the random number at each iteration, diffusion may occur in later steps even within the same pair.

Steady-state binary diffusion

For a case study, the steady-state binary diffusion across a two-dimensional plane sheet was considered. An $H \times L$ lattice was initialized, as shown in Fig. 4a, such that the first column represented a source at $C_{1,\text{source}} = 1$, while the last column represented a sink at $C_{1,\text{sink}} = 0$. The system was assumed to be constrained by a non-permeable boundary. Steady state was defined as the point where the average concentration profiles did not change with time. Simulations were run for 15,000 time steps, and were repeated 10 times to obtain averaged profiles.

The analytical solution from Crank²⁸ for variable diffusion coefficients is given by:

$$\frac{C_{1,\text{source}} + F(C_{1,\text{source}}) - C_1 - F(C_1)}{C_{1,\text{source}} + F(C_{1,\text{source}}) - C_{1,\text{sink}} - F(C_{1,\text{sink}})} = \frac{x}{l} \quad (9)$$

$$F(C_1) = \int_0^{C_1} f(C'_1) dC'_1 \quad (10)$$

where $l = L - 2 = 38$ is the distance between the faces of the plane sheet excluding the boundary cells, x is the column number, $D_0 = 1$ is the reference diffusion coefficient, and $D(C_1) = D_0(1 + f(C_1))$. For instance, with $f(C_1) = -0.5C_1$, the solution reduces to:

$$C_1(x) = 2 - \sqrt{1 + \frac{3x}{l}} \quad (11)$$

At the sink side ($C_{1,\text{sink}} = 0$), i.e., $D = 1$, there is a maximum diffusion probability of 1, whereas at the source side ($C_{1,\text{source}} = 1$), $D = 0.5$, corresponding to a probability of 0.5.

Non-steady-state binary diffusion

To study the non-steady-state diffusion, an $H \times L$ lattice was split into two halves separated by a door, as shown in Fig. 5a. One half was filled with substance 1 and the other half with substance 2. At time $t = 0$, the door was opened, initiating diffusion in a closed system. Simulations were run for 15,000 iterations until equilibrium, and were repeated 10 times. For this case, the probability of a diffusion event was mapped directly to the experimental binary ethanol-water diffusion coefficients. The diffusion coefficient data at 25 °C from Pratt et al.²⁹ were normalized between 0 and 1, from which the $D(C_{1,\text{norm}})$ was defined as:

$$D(C_{1,\text{norm}}) = \frac{D(C_1)}{D_{\max}} = p(C_1) \quad (12)$$

The dependence of experimental D on ethanol mole fraction C_1 was fitted to a quartic polynomial function, as shown in Fig. 6:

$$p(C_1) = 6.19C_1^4 - 17.36C_1^3 + 17.17C_1^2 - 6.13C_1 + 1.00 \quad (13)$$

This equation allowed diffusion to be modeled with concentration-dependent transport probabilities, which provide a closer agreement with experimental binary solvents diffusion behavior.

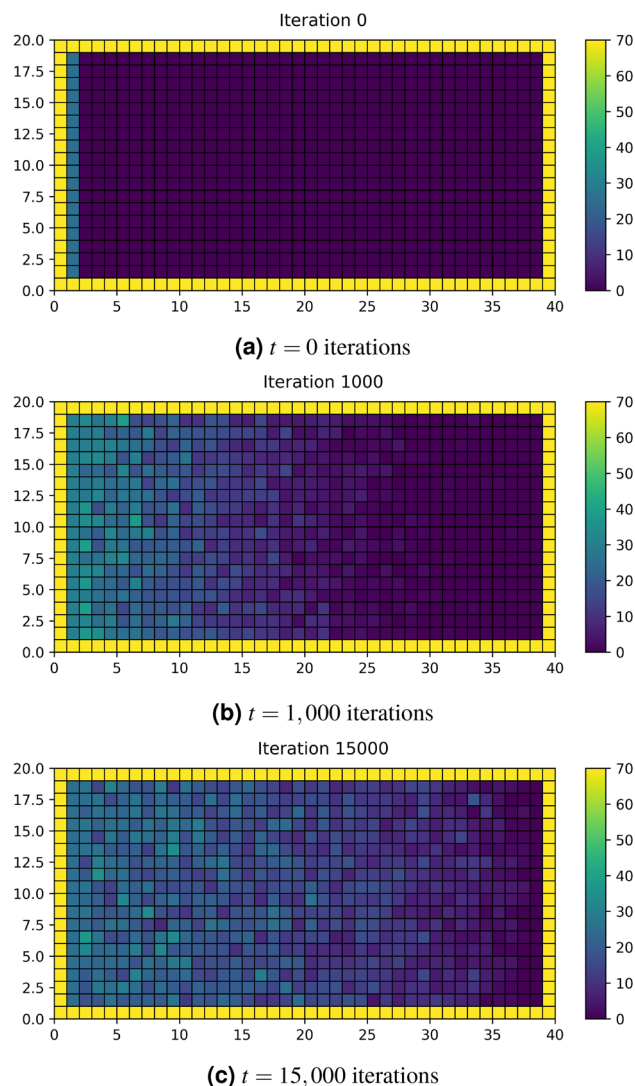


Fig. 4. Binary diffusion of substance 1 (nonsolvent) and substance 2 (solvent) on a two-dimensional plane sheet of dimensions $H = 20$, $L = 40$, with source and sink at the extreme ends. The yellow cells represent the non-permeable boundary. The color scale denotes the number of molecules in the cells. The images represent the snapshots from one simulation.

Results and discussion

Single component diffusion

The non-steady-state diffusion in single component systems arising from two instantaneous sources: Case 1 line source and Case 2 point source was investigated. Concentration profiles as a function of distances from the center of the lattices were analyzed and compared with known analytical solutions. The concentration-distance curves as seen from Fig. 7 demonstrate excellent agreement between the model-predicted data points from this work and the analytical solutions from Eqs. 3 and 5 respectively. For both line and point sources, the average concentration number on the y-axis of Fig. 7 is the ratio of the number of molecules in each column (C) over the total number of molecules in all the cells of the lattice (A). The agreement between the simulated and analytical concentration profiles for both the line and point sources, as seen from Fig. 7, confirms that the stochastic exchange rule shows Fickian behavior independent of the initial spatial distribution of molecules.

The distinction between the different sources in diffusion arises from their initial spatial distribution. The line source disperses the molecules along a single axis of the lattice, which results in an initial concentration profile that is spatially extended. This configuration leads to a lower maximum concentration at the outset cells. In contrast, the point source has all molecules at a single lattice cell, which causes an extremely high initial local concentration and results in a steep gradient from the origin.

The differences in the concentration profiles as seen from Fig. 7 highlight the effect of source geometry and stochastic effects inherent in the model. When all molecules are initially concentrated at a single cell, as with the point source, individual molecular trajectories have a substantial impact on local concentration, particularly near the origin. This introduces larger fluctuations, which are seen as higher standard deviations in the measured

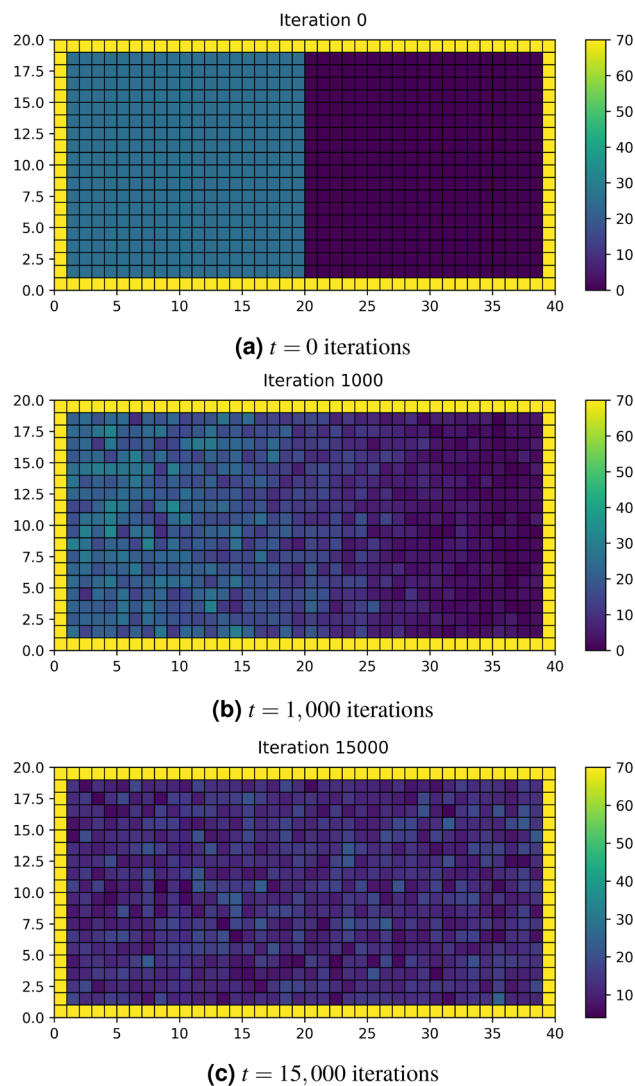


Fig. 5. Binary diffusion of substance 1 (nonsolvent) and substance 2 (solvent) based on a sliding door approach on a two-dimensional lattice with dimensions $H = 20$, $L = 40$. The color scale denotes the number of molecules in the cells. The images represent the snapshots from one simulation.

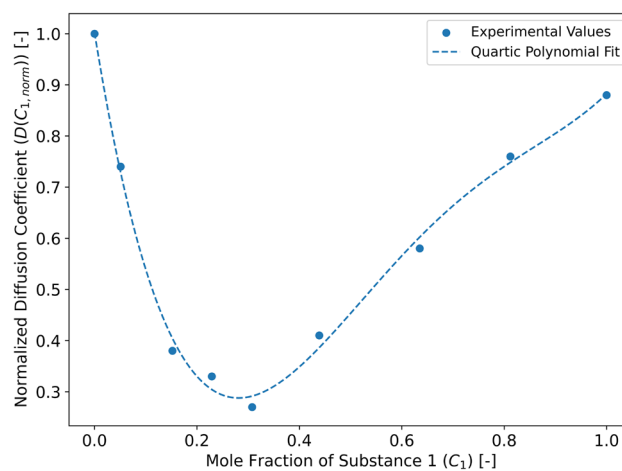


Fig. 6. The experimental data from Pratt et al.²⁹ for concentration-dependent diffusion coefficient of ethanol-water mixtures is normalized and fitted to a quartic polynomial function with the $R^2 = 0.99$.

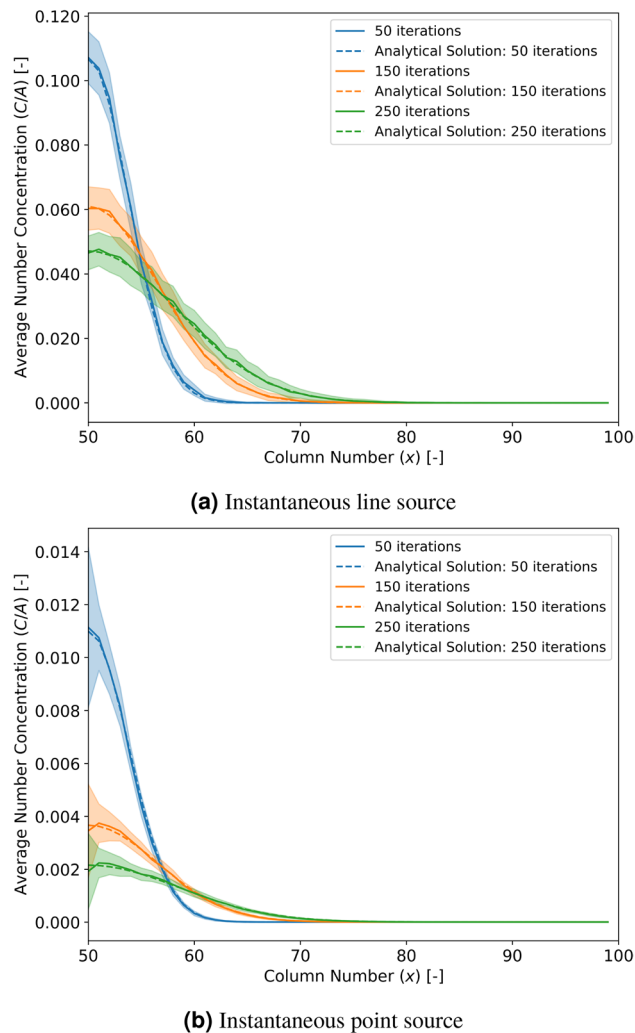


Fig. 7. The concentrations profiles against the distance from the origin of the source for different lengths of time steps. The solid lines represent the simulation and the dotted lines represent the fit from the analytical solution. The standard deviations ($n = 10$) are represented as bands.

profiles. From Fig. 7a, the line source, with its distributed initialization, averages out stochastic variations across the cells, which results in lower standard deviations as compared to the point source from Fig. 7b. A practical consequence is that geometries similar to the point source configurations require a larger number of repeated simulations, or larger lattice sizes, to achieve comparable statistical precision to line source configurations at higher computational cost.

In this version of the model, the simulated concentration profiles were fitted to the analytical solutions from Crank to quantify the diffusion coefficient D . A comparison of the diffusion coefficients for both the instantaneous line and point sources is shown in Fig. 8. The results show that the diffusion coefficients from the point source exhibit greater standard deviation at each length of the time step compared to the line source. This is consistent with the increased fluctuations due to the stochastic nature near the source.

Despite these differences in local variability and spatial gradients, both cases converge to yield diffusion coefficients of similar magnitude (around $0.14 \frac{\text{cells}^2}{\text{timestep}}$) and remain consistent over different time steps.

This underlines the Fickian nature of the diffusion process captured by the cellular automata framework. This convergence confirms the accuracy and reliability of the model for simulating non-steady-state diffusion phenomena in systems with differing initial spatial geometries. This is consistent with the analysis of Chopard and Droz¹⁵, who showed that macroscopic diffusive transport emerges from a probabilistic cellular automaton regardless of microscopic initial conditions, provided the exchange rule itself is unbiased between neighboring cells. It is worth noting, however, that this agreement reflects a shared conclusion rather than a shared mechanism: the model of Chopard and Droz is built on an exclusion-principle random walk with an exact discrete Boltzmann equation, whereas the present PCA framework uses stochastic exchange governed by a maximum cell occupancy rather than a directional exclusion principle, without an equivalent closed-form kinetic description. The

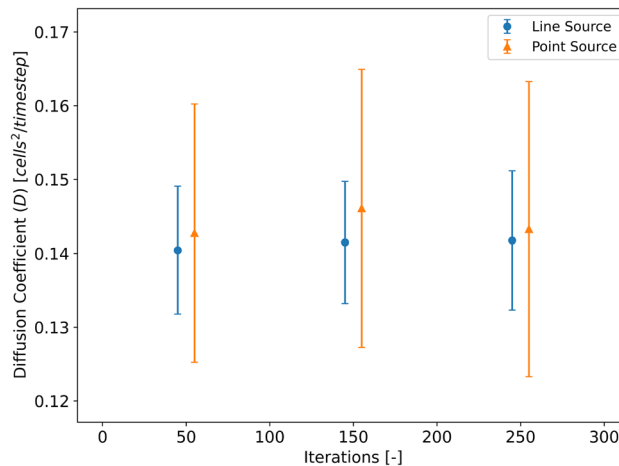


Fig. 8. Comparison of diffusion coefficients calculated from the single component diffusion from the instantaneous line and point sources. The standard deviations are calculated based on $n = 10$ simulations.

agreement in emergent Fickian behavior therefore validates the macroscopic correctness of the present model rather than implying that the two microscopic mechanisms are equivalent.

With numerical diffusion coefficient $D_{\text{numerical}}$ being $0.14 \frac{\text{cells}^2}{\text{time step}}$, the characteristic time scale τ , obtained using ($D_{\text{numerical}}$), the lattice cell length r , and the experimental diffusion coefficient of water ($D_{\text{experimental}}$), obtained from Krynicki et al.³⁰, is calculated as follows:

$$\begin{aligned}\tau &= \frac{D_{\text{numerical}} \cdot r^2}{D_{\text{experimental}}} \\ &= \frac{0.14 \cdot (10^{-9} \text{ m})^2}{2.3 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}} \approx 6.1 \times 10^{-11} \text{ s}\end{aligned}\quad (14)$$

Therefore, 1000 iterations roughly represent the changes seen at a temporal scale of 61 ns. This mapping allows the number of lattice time steps used throughout this work to be interpreted in terms of real experimental timescales.

Binary component diffusion

Steady-state binary diffusion

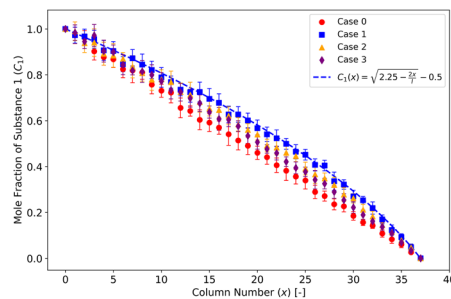
To determine the correct probability of diffusion events to happen as a function of local concentration of the molecules, the steady-state binary diffusion case was employed. Three cases of probability functions as mentioned in Eqs. 6, 7, 8 were tested in a source-sink lattice, which is seen from Fig. 4a.

To assess the performance of each probability function, the simulated concentration profiles were compared with the analytical solutions, as shown in Fig. 9. These analytical solutions depend differently on the diffusion coefficients. Fig. 9a shows the obtained concentration profile from the use of different probability functions and the analytical solution from Crank²⁸. From Fig. 9b, it is clear that the Case 1, described in Eq. 6, has the closest agreement with the analytical solution. From this, we can understand the role of averaging the local concentration in capturing the nonlinear binary diffusion; this diffusion is governed by the composition shared between the two exchanging cells, rather than by the state of either cell alone. This is conceptually analogous to Fick's second law with a concentration-dependent diffusivity, where the local flux depends on the composition at the point of exchange rather than being biased toward the higher or lower concentration side.

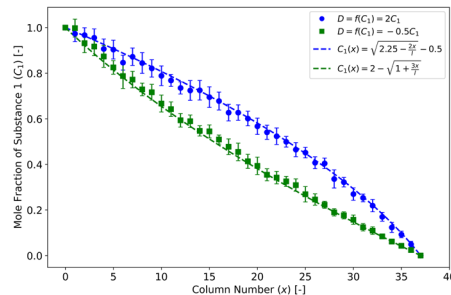
On the other hand, the Case 0, which represents the single component diffusion with constant D , further clarifies the impact of the probability function. When diffusion events are independent of local composition, the model produces linear concentration profiles because of the constant diffusion coefficient and no interaction. The binary diffusion case takes into consideration a concentration-dependent diffusion probability $p(C_1)$, as shown in Fig. 6 for the ethanol-water system. This leads to distinctly nonlinear profiles, which reflect the experimental observations and the theoretical expectations. This resulting deviation from the linear behavior indicates that the model is successful in translating compositional effects into diffusion behavior.

Non-steady-state binary diffusion

In order to further validate the cellular automata modeling approach for binary diffusion, a non-steady-state was examined in which a two-component system of ethanol (substance 1) and water (substance 2) initially separated by a sliding door was permitted to diffuse within a closed two-dimensional lattice. Following the opening of the door at time $t = 0$, the progression of ethanol distribution was monitored at discrete time intervals up to 15,000 iterations.



(a) Probability functions of Case 0, 1, 2 and 3 compared with analytical solution from Crank²⁸.



(b) Probability function of Case 1 compared with two analytical solutions from Crank²⁸.

Fig. 9. Comparison of binary diffusion probability functions with analytical solutions. The standard deviations are calculated based on $n = 10$ simulations.

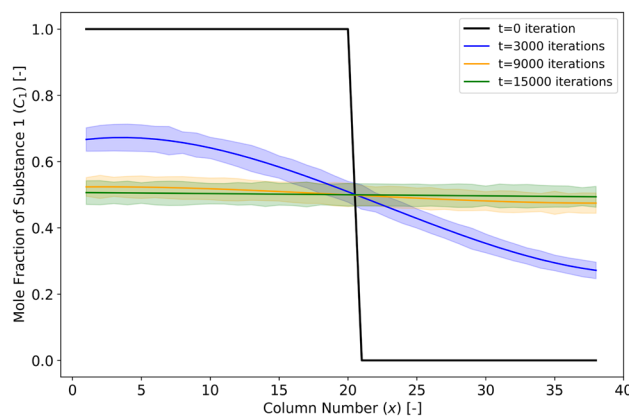


Fig. 10. Mole fraction of substance 1 (ethanol) along the length of the lattice for $t = 0$, $t = 3,000$, $t = 9,000$ and $t = 15,000$ iterations. The standard deviations ($n = 10$) are represented as bands.

Fig. 10 captures the temporal development of the ethanol concentration profile across the lattice. During the initial stages (around 3,000 iterations), the profile is characterized by a pronounced gradient and the elevated local changes. This reflects the sudden transition imposed by the sliding door and inherently stochastic nature of the simulation. As the diffusion progressed, the magnitude of the concentration gradient reduced and the spatial profile approached uniformity.

By 15,000 iterations, the system achieved equilibrium, marked by a flat concentration profile, at a value near 0.5, which is half of the ethanol concentration. This result clearly indicates that the lattice space is evenly partitioned between ethanol and water, signifying the effective diffusion-driven equilibration in the closed system. The evolution depicted in Fig. 10 not only corroborates the validity of the cellular automata approach for non-steady-state binary diffusion but also showcases its utility for modeling transient molecular distributions and equilibration in multi-component porous systems.

Conclusion

This study presents a two-dimensional probabilistic cellular automata (PCA) model for molecular diffusion in single and binary component systems. By generalizing Vanag's PCA framework to incorporate a concentration-dependent diffusion probability, the model effectively transcends limitations of constant diffusion coefficients and captures composition-dependent transport behavior in the specific test geometries examined in the work.

The method successfully reproduces classical analytical solutions for non-steady-state and steady-state diffusion from different source geometries. This validates the accuracy and demonstrates the spatial and temporal concentration profiles with stochastic fluctuations and boundary effects.

The dependence of the exchange probability on the local composition of two neighboring cells was tested using three different rules, each compared against Crank's analytical solution for diffusion with a variable diffusion coefficient. This comparison identified the rule that most accurately reproduces the corresponding macroscopic, nonlinear concentration profile.

The model further adopts a synchronous, Margolus block-partitioned scheme in place of Vanag's original asynchronous formulation, without loss of agreement with the analytical solutions for either single or binary component diffusion.

The validation cases considered serve primarily to establish the correctness of the concentration-dependent exchange rule introduced in this work. Building on the validated model, our companion manuscript²⁶ introduces polymer fibers that establish a mechanistic link between molecular transport and the dynamic microstructure of elastic gels, allowing the diffusive lattice and the evolving fiber network to be updated together on the same discrete structure without remeshing. This multiscale coupling enhances the understanding of gel swelling, phase behavior, and solvent interactions, which are critical for material design, and is where the present framework offers a practical advantage over grid-based continuum solvers. Extending the present two-dimensional formulation to three dimensions, and deriving the composition-dependent exchange probability from an underlying thermodynamic quantity rather than from calibration to experimental data, remain directions for future work.

Data availability

The code supporting the findings of this study is available in the supplementary information: <https://doi.org/10.5281/zenodo.20345641>.

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Declarations

Competing interests

The authors declare no competing interests.

Additional information

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