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Collision-mediated Transfer Kinetics of Cargo Among Mobile Nanocarriers

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Abstract

Micelles, liposomes, microgels, dendrimers, macrocyclic host molecules, and nanoparticles represent nanocarriers used to transfer cargo—such as drug molecules—among each other and to target sites. We calculate the kinetics of collision-mediated transfer of cargo within ensembles of chemically distinct mobile nanocarriers that each hosts non-interacting cargo items on discrete and identical sites. Rate equations for collision-mediated transfer of cargo are expressed in the Gaussian limit as a set of Fokker-Planck equations and solved in the limit of low occupation. The results are analytic expressions for the detailed cargo distributions of each carrier type as a function of time, from an arbitrary initial apportionment to a set of Gaussians in equilibrium.

The transport of cargo through mobile nanocarriers (NCs) is ubiquitous in living systems and utilized in pharmaceutical and technological applications such as drug delivery [1], food science [2], dry powder coating [3], and host-guest complexes [4]. When being used as carriers, liposomes, polymersomes, colloidosomes [5], microcapsules, micelles, nanoshells, microgels, dendrimers, and nanoparticles [6, 7] often allow for their cargo to be released and taken up by another type of carrier, either through a diffusion mechanism or directly upon carrier-carrier collisions [8]. Measuring and modeling the resulting transport kinetics has yielded insights into the physical mechanisms and characteristic time scales of liposomal drug delivery [8–11].

In the present work, we advance and generalize existing models [10–12] for the kinetics of cargo transfer to the presence of multiple, chemically distinct types of NCs. Starting from a general set of rate equations governing collision-mediated cargo transfer among NCs, we transition to the Gaussian regime, where we focus on low occupation numbers. This leads to a set of Fokker-Planck equations, which we solve analytically to predict how the cargo distributions of all carrier types jointly evolve from arbitrary initial states to their specific Gaussian equilibrium distributions. Applications of our model include supromolecular nanocarriers [4] that exchange their load through collisions such as liposomes and other amphiphile-based nanoparticles used for the delivery of poorly water-soluble drugs [13], assemblies of colloidal particles [14], and the transfer of fine particles between carriers in dry powder coating [3, 15].

Consider a unit volume that contains L different types of mobile NCs, all uniformly distributed. Type l (with $1 \leq l \leq L$) is present with a fixed number of N_l individual NCs that each can host up to m_l cargo items. Fig. 1 shows an illustration with NCs belonging to four different types, each containing a different distribution of cargo items. We describe cargo distributions by the numbers $y_l^{(i)} = y_l^{(i)}(t)$ of NCs of type l that contain i cargo items at time t . The distributions satisfy the conservation requirements $N_l = \sum_{i=0}^{m_l} y_l^{(i)}$. The total number of all cargo items, $M = \sum_{l=1}^L M_l(t)$, carried collectively by all NCs is fixed, but the total numbers hosted by each NC type, $M_l(t) = \sum_{i=0}^{m_l} i y_l^{(i)}$, may vary in time. We allow cargo items to change their host when two NCs collide and employ chemical reaction kinetics to characterize the corresponding transfer process. This involves a set of positive rate constants K_{kl} (with $1 \leq k \leq L$ and $1 \leq l \leq L$) that characterize the nominal probability of a cargo item to move from a k -type to an l -type NC upon collision. Kinetic equations for the rate

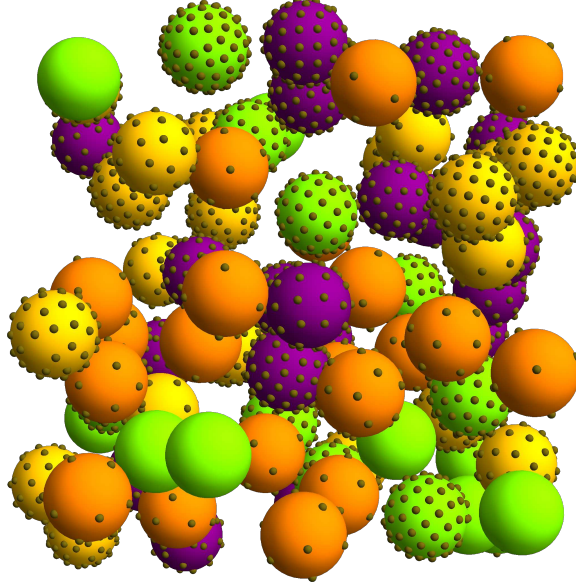


FIG. 1: Illustration of NCs belonging to four distinct types, marked by four different colors, and cargo items represented by bulging dark dots on the surfaces of the NCs. Distributions of cargo among NCs of each type are assigned arbitrarily.

of change of $y_l^{(i)}$,

$$\begin{aligned} \frac{dy_l^{(i)}}{dt} = & \sum_{k=1}^L \left[K_{kl} \sum_{j=0}^{m_k} \left(g_{m_l}^{j \rightarrow (i-1)} y_l^{(i-1)} - g_{m_l}^{j \rightarrow i} y_l^{(i)} \right) y_k^{(j)} \right. \\ & \left. + K_{lk} \sum_{j=0}^{m_k} \left(g_{m_k}^{(i+1) \rightarrow j} y_l^{(i+1)} - g_{m_k}^{i \rightarrow j} y_l^{(i)} \right) y_k^{(j)} \right] \end{aligned} \quad (1)$$

honor all relevant collisions. They employ the definitions $y_l^{(-1)} = y_l^{(m_l+1)} = 0$ and apply to all l and i with $1 \leq l \leq L$ and $0 \leq i \leq m_l$. Let us use the notation NC_l^i for an individual l -type NC that contains i cargo items. The four distinct types of terms on the right-hand side of Eq. 1 then describe addition of a cargo item to NC_l^{i-1} and NC_l^i as well as removal of a cargo item from NC_l^{i+1} and NC_l^i . We assume each NC_l^i has its i cargo items distributed randomly over the available m_l sites and that all sites are identical, in contrast to the case of non-identical sites that reflect non-spherical carrier geometry and/or non-uniform distribution of cargo items on or inside the carrier [16]. Each term in the rate equations then includes a factor

$$g_{m_k}^{i \rightarrow j} = m_l \frac{\binom{m_l-1}{i-1} \binom{m_k-1}{j}}{\binom{m_l}{i} \binom{m_k}{j}} = i - \frac{ij}{m_k} \quad (2)$$

that accounts for the random statistical occurrence of all possible cargo distributions in a

transfer event from NC_l^i to NC_k^j . For example, if the accepting NC is completely filled with cargo, $j = m_k$, then no transfer is possible, implying $g_{m_k}^{i \rightarrow j} = 0$. Previous analyses of Eqs. 1-2 have focused exclusively on the case $L = 1$ [12, 17, 18].

To find the total numbers of cargo items hosted by type- l NCs, $M_l(t)$, we compute the first moment $dM_l/dt = \sum_{i=0}^{m_l} i(dy_l^{(i)}/dt)$ with $dy_l^{(i)}/dt$ specified in Eq. 1, yielding L non-linear differential equations,

$$\begin{aligned} \frac{dM_l(t)}{dt} = & \sum_{k=1}^L \left[K_{kl} N_l - \delta_{kl} \left(\sum_{n=1}^L K_{ln} N_n \right) \right. \\ & \left. + \left(\frac{K_{lk}}{m_k} - \frac{K_{kl}}{m_l} \right) M_l(t) \right] M_k(t), \end{aligned} \quad (3)$$

with the Kronecker delta $\delta_{kl} = 0$ for $k \neq l$ and $\delta_{kl} = 1$ for $k = l$. In equilibrium, for $t \rightarrow \infty$, the exact solution of Eq. 1 is a set of binomial distributions

$$y_l^{(i)}(t \rightarrow \infty) = N_l \binom{m_l}{i} \left(\frac{\bar{\mu}_l}{m_l} \right)^i \left(1 - \frac{\bar{\mu}_l}{m_l} \right)^{m_l-i}, \quad (4)$$

where $\bar{\mu}_l = \mu_l(t \rightarrow \infty)$ is the long-time limit of the instantaneously preferred number of cargo items per NC

$$\mu_l(t) = \frac{1}{\zeta_l(t)} \sum_{k=1}^L K_{kl} M_k(t) \quad (5)$$

with an effective, time-dependent rate constant

$$\zeta_l(t) = \sum_{k=1}^L \left[K_{lk} N_k + \left(\frac{K_{kl}}{m_l} - \frac{K_{lk}}{m_k} \right) M_k(t) \right] \quad (6)$$

that characterizes the entire transfer of type- l NCs. Our focus in this work is on NCs that carry large numbers of cargo items. In this case, we can transition to a continuum description, replacing the discrete distributions $y_l^{(i)} = y_l^{(i)}(t)$ by continuous distributions $y_l = y_l(x, t)$, namely the number of NCs of type l per unit volume that carry x cargo items at time t . The condition $1 \ll \mu_l(t) \ll m_l$ defines the *Gaussian regime*, in which the kinetic equations in Eq. 1 turn into a set of coupled Fokker-Planck equations

$$\frac{1}{\zeta_l(t)} \frac{\partial y_l}{\partial t} = \frac{\partial}{\partial x} \{ [x - \mu_l(t)] y_l \} + \mu_l(t) \left[1 - \frac{\mu_l(t)}{m_l} \right] \frac{\partial^2 y_l}{\partial x^2} \quad (7)$$

and the binomial distributions in Eq. 4 become Gaussians

$$y_l(x, t \rightarrow \infty) = \frac{N_l}{\sqrt{2\pi\bar{\mu}_l(1 - \bar{\mu}_l/m_l)}} e^{-\frac{(x - \bar{\mu}_l)^2}{2\bar{\mu}_l(1 - \bar{\mu}_l/m_l)}}. \quad (8)$$

Because the equilibrium solutions of Eq. 1 are given by Eq. 4, those of Eq. 7 must correspond to Eq. 8 [19]. This is indeed the case. Note that Eq. 7 conserves $N_l = \int_{-\infty}^{\infty} dx y_l(x, t)$ and produces Eq. 3 from the first moment $M_l(t) = \int_{-\infty}^{\infty} dx x y_l(x, t)$. Eqs. 7 constitute a general framework to describe the transfer kinetics of cargo in the Gaussian regime. Solutions can easily be obtained for $L = 1$. Progress toward finding analytic solutions for any choice of L can be made in the limit of *low occupation*, where $m_l \rightarrow \infty$ implies $\mu_l(t) \ll m_l$, and $\zeta_l(t) = \zeta_l$ with $\zeta_l = \sum_{k=1}^L K_{lk} N_k$ is no longer time-dependent. The resulting set of Fokker-Planck equations

$$\frac{1}{\zeta_l} \frac{\partial y_l}{\partial t} = \frac{\partial}{\partial x} \{ [x - \mu_l(t)] y_l \} + \mu_l(t) \frac{\partial^2 y_l}{\partial x^2} \quad (9)$$

are equivalent to the kinetic equations in Eq. 1 in the limit of low occupation, yet not too low so that the continuum description remains valid. Eqs. 1 can be viewed as Master equations that can be represented by Fokker-Planck equations for continuously changing stochastic variables $y_l^i(t) \rightarrow y_l(x, t)$. Typically, for example in the kinetic theory of mass transfer [20], transition probabilities can be linked to interaction potentials between particles. In contrast, our present work introduces *ad hoc* a set of constant transition probabilities, namely the rate constants K_{ij} . Before solving Eq. 9 analytically, we note that from Eq. 9 we obtain the differential equation

$$\frac{dM_l(t)}{dt} = \zeta_l [N_l \mu_l(t) - M_l(t)] = \sum_{k=1}^L R_{lk} M_k(t) \quad (10)$$

for the total number of cargo items $M_l(t) = \int_{-\infty}^{\infty} dx x y_l(x, t)$ carried by NCs of type l . The right-hand side of Eq. 10 defines the *rate matrix* [21]

$$R_{lk} = K_{kl} N_l - \delta_{kl} \times \sum_{n=1}^L K_{ln} N_n, \quad (11)$$

an $L \times L$ square matrix with all nondiagonal elements $R_{lk} = K_{kl} N_l$ being positive and real-valued and all diagonal elements $R_{ll} = -\sum_{n=1, n \neq l}^L K_{ln} N_n$ the negative of the sum of all nondiagonal elements in the corresponding matrix column. That is, the sum of all elements in each column vanishes. The rate matrix R_{lk} has a set of $L-1$ eigenvalues $\{\lambda_1, \lambda_2, \dots, \lambda_{L-1}\}$ that all have a non-positive real part, and one vanishing eigenvalue $\lambda_L = 0$. Pairs of complex conjugate eigenvalues may be present, all other eigenvalues are real-valued [22]. The solution of Eq. 10 can be written as $M_l(t) = \sum_{n=1}^L c_n b_{ln} e^{\lambda_n t}$, where the b_{ln} are the eigenvectors of the rate matrix and the c_n constant coefficients, chosen to satisfy a given set of initial conditions

$M_l(t = 0)$. We thus find $\mu_l(t) = \bar{\mu}_l + \sum_{n=1}^{L-1} W_{ln} e^{\lambda_n t}$ with $W_{ln} = (c_n/\zeta_l) \sum_{k=1}^L K_{kl} b_{kn}$. We also note that $\bar{\mu}_l = W_{lL} = M_l(\infty)/N_l$.

With $\mu_l(t)$ known, we proceed toward solving Eq. 9. Transforming that equation into Fourier space through $\tilde{y}_l(k, t) = \int_{-\infty}^{\infty} dx y_l(x, t) e^{-ikx}$ affords the solution

$$\tilde{y}_l(k, t) = \tilde{f}_l(k e^{-\zeta_l t}) \times e^{-\int_{k e^{-\zeta_l t}}^k d\bar{k} (\bar{k} + i) \mu_l\left(t + \frac{1}{\zeta_l} \ln \frac{\bar{k}}{k}\right)}, \quad (12)$$

where $\tilde{f}_l(k) = \tilde{y}_l(k, t = 0)$ are the Fourier transforms of the initial distributions $f_l(x) = y_l(x, t = 0)$. In the long time limit, $t \rightarrow \infty$, we obtain $\tilde{y}_l(k, t \rightarrow \infty) = N_l \exp[-\bar{\mu}_l k(i + k/2)]$ and from this the Gaussian distributions $y_l(x, t \rightarrow \infty) = N_l \exp[(x - \bar{\mu}_l)^2/(2\bar{\mu}_l)]/\sqrt{2\pi\bar{\mu}_l}$. Note that the integral

$$-\int_{k e^{-\zeta_l t}}^k d\bar{k} (\bar{k} + i) \left[\mu_l\left(t + \frac{1}{\zeta_l} \ln \frac{\bar{k}}{k}\right) - \bar{\mu}_l \right] = ikP_l(t) + \frac{k^2}{2}Q_l(t) \quad (13)$$

is quadratic in k with time-dependent coefficients

$$\begin{aligned} P_l(t) &= -\sum_{n=1}^{L-1} \frac{W_{ln}\zeta_l}{\lambda_n + \zeta_l} (e^{\lambda_n t} - e^{-\zeta_l t}), \\ Q_l(t) &= -2\sum_{n=1}^{L-1} \frac{W_{ln}\zeta_l}{\lambda_n + 2\zeta_l} (e^{\lambda_n t} - e^{-2\zeta_l t}) \end{aligned} \quad (14)$$

that vanish initially, $P_l(t = 0) = Q_l(t = 0) = 0$, and in the long-time limit, $P_l(t \rightarrow \infty) = Q_l(t \rightarrow \infty) = 0$. To transform the solution in Eq. 12 back to real space, we express the Fourier transform of the initial distribution

$$\tilde{f}_l(k) = N e^{-\bar{\mu}_l\left(ik + \frac{k^2}{2}\right)} \times \int_{-\infty}^{\infty} d\bar{x} a_l(\bar{x}) e^{-ik\bar{x}} \quad (15)$$

as the product of the Fourier transform of $y_l(x, t \rightarrow \infty)$ and the Fourier transform of a function $a_l(\bar{x})$ that we demand to have fixed zeroth and first moments,

$$\int_{-\infty}^{\infty} d\bar{x} a_l(\bar{x}) = 1, \quad \int_{-\infty}^{\infty} d\bar{x} \bar{x} a_l(\bar{x}) = \frac{M_l(0)}{N_l} - \bar{\mu}_l \quad (16)$$

to conserve N_l and produce given initial conditions $M_l(t = 0)$. The latter also demands a total vanishing first moment $\int_{-\infty}^{\infty} d\bar{x} \bar{x} \sum_{l=1}^L a_l(\bar{x}) = 0$ to conserve $M = \sum_{l=1}^L M_l(t)$. Using

Eqs. 12-15 leads to the expression

$$y_l(x, t) = N_l \frac{\int_{-\infty}^{\infty} d\bar{x} a_l(\bar{x}) e^{-\frac{1}{2} \frac{(\bar{\mu}_l - P_l(t) - x + \bar{x} e^{-\zeta_l t})^2}{\bar{\mu}_l - Q_l(t)}}}{\sqrt{2\pi(\bar{\mu}_l - Q_l(t))}} \quad (17)$$

for the solutions of Eq. 9. As demanded, $y_l(x, t)$ in Eq. 17 conserves $N_l = \int_{-\infty}^{\infty} dx y_l(x, t)$. When calculating the number of cargo items $M_l(t) = \int_{-\infty}^{\infty} dx x y_l(x, t)$ in NCs of type l , we find $M_l(t) = M_l(\infty) + e^{\zeta_l t} [M_l(0) - M_l(\infty)] - N_l P_l(t)$, which indeed solves Eq. 10. The expression for the initial distributions $f_l(x) = y_l(x, t=0)$ that follows from Eq. 17,

$$f_l(x) = \frac{N_l}{\sqrt{2\pi\bar{\mu}_l}} \int_{-\infty}^{\infty} d\bar{x} a_l(\bar{x}) e^{-\frac{1}{2} \frac{(x - \bar{\mu}_l - \bar{x})^2}{\bar{\mu}_l}}, \quad (18)$$

are Weierstrass transforms of $a_l(x)$; the inverse transform

$$a_l(x) = \frac{1}{N_l} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\bar{\mu}_l}{2}\right)^2 H_n\left(\frac{x}{\sqrt{2\bar{\mu}_l}}\right) \left(\frac{d^n f_l(x)}{dx^n}\right)_{x=\bar{\mu}_l} \quad (19)$$

allows us, in principle, to find the functions $a_l(x)$ in terms of the n -th derivatives $d^n f_l(x)/dx^n$ of $f_l(x)$ at the position $x = \bar{\mu}_l$. Here, $H_n(z)$ denotes the n -th order Hermitian polynomial. Eq. 17, which is a major result of this work, represents the complete solution of the differential equations in Eq. 9 for each l -type NC and corresponding initial distribution $f_l(x)$. The emergence of $f_l(x)$ has been discussed by Wittmann *et al* [23].

For certain types of initial distributions $f_l(x)$ it is convenient to re-express the solution in Eq. 17. We discuss two alternative representations. The first is based on the relation $e^{2z_l b_l - b_l^2} = \sum_{n=0}^{\infty} H_n(z_l) b_l^n / n!$ with

$$\begin{aligned} z_l &= z_l(x, t) = \frac{x - \bar{\mu}_l + P_l(t)}{\sqrt{2(\bar{\mu}_l - Q_l(t))}}, \\ b_l &= b_l(x, t) = \frac{\bar{x} e^{-\zeta_l t}}{\sqrt{2(\bar{\mu}_l - Q_l(t))}}. \end{aligned} \quad (20)$$

This leads to an equivalent representation of the solution as

$$y_l(x, t) = N_l \frac{e^{-z_l(x, t)^2}}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{c_n^{(l)} e^{-n\zeta_l t} H_n(z_l(x, t))}{n! [2(\bar{\mu}_l - Q_l(t))]^{\frac{n+1}{2}}}, \quad (21)$$

where the coefficients

$$\begin{aligned} c_n^{(l)} &= \int_{-\infty}^{\infty} d\bar{x} \bar{x}^n a_l(\bar{x}) \\ &= \frac{1}{N_l} \left(\frac{\bar{\mu}_l}{2}\right)^{\frac{n}{2}} \int_{-\infty}^{\infty} dx f_l(x) H_n\left(\frac{x - \bar{\mu}_l}{\sqrt{2\bar{\mu}_l}}\right) \end{aligned} \quad (22)$$

appear as moments of the functions $a_l(\bar{x})$ or can be calculated directly from the initial distributions $f_l(x)$. We demand $c_0^{(l)} = 1$ and $c_1^{(l)} = M_l(0)/N_l - \bar{\mu}_l$ to conserve N_l and reproduce $M_l(0)$, respectively, as well as $\sum_{l=1}^L c_1^{(l)} = 0$ to conserve M .

The second alternative representation assumes the function

$$a_l(\bar{x}) = \frac{1}{\sqrt{2\pi}} \sum_{i=1}^{n_l} \frac{\theta_i^{(l)}}{\sqrt{\gamma_i^{(l)}}} e^{-\frac{1}{2} \frac{(\bar{x} - \eta_i^{(l)})^2}{\gamma_i^{(l)}}}, \quad (23)$$

to be the sum of n_l Gaussian distributions, each involving a fraction $\theta_i^{(l)} = N_l^{(i)}/N_l$ of l -type carriers so that $\sum_{i=1}^{n_l} \theta_i^{(l)} = 1$. The peak locations $\eta_i^{(l)}$ determine the initial cargo item content in l -type NCs through $\sum_{i=1}^{n_l} \theta_i^{(l)} \eta_i^{(l)} = M_l(0)/N_l - \bar{\mu}_l$ and must satisfy $\sum_{l=1}^L N_l \sum_{i=1}^{n_l} \theta_i^{(l)} \eta_i^{(l)} = 0$ to conserve M . Eq. 23 yields

$$y_l(x, t) = \frac{N_l}{\sqrt{2\pi}} \sum_{i=1}^{n_l} \frac{\theta_i^{(l)} e^{-\frac{1}{2} \frac{(x - \bar{\mu}_l + P_l(t) - \eta_i^{(l)} e^{-\zeta_l t})^2}{\bar{\mu}_l - Q_l(t) + \gamma_i^{(l)} e^{-2\zeta_l t}}}}{\sqrt{\bar{\mu}_l - Q_l(t) + \gamma_i^{(l)} e^{-2\zeta_l t}}} \quad (24)$$

and thus reveals that an arbitrary number of initially Gaussian distributions of the carrier items

$$f_l(x) = \frac{N_l}{\sqrt{2\pi}} \sum_{i=1}^{n_l} \frac{\theta_i^{(l)} e^{-\frac{1}{2} \frac{(x - \bar{\mu}_l - \eta_i^{(l)})^2}{\bar{\mu}_l + \gamma_i^{(l)}}}}{\sqrt{\bar{\mu}_l + \gamma_i^{(l)}}} \quad (25)$$

remain Gaussian at all time until reaching the equilibrium distribution $y_l(x, t \rightarrow \infty) = (N_l/\sqrt{2\pi\bar{\mu}_l}) \times e^{-(x - \bar{\mu}_l)^2/(2\bar{\mu}_l)}$.

In the presence of a single NC type ($L = 1$), all transfer remains internal within the same type of carrier, implying fixed $M_1(t) = M$ and $\mu_1(t) = \bar{\mu}_1 = M/N_1$. The functions $P_1(t) = Q_1(t) = 0$ both vanish identically, and $1/\zeta_1 = 1/(K_{11}N_1)$ defines the only existing characteristic time. We exemplify the behavior of $y_1(x, t)$ by adding $N_1/2$ empty carriers at $t = 0$ to $N_1/2$ carriers that contain a pre-equilibrated distribution of M cargo items. This corresponds to choosing $n_1 = 2$ as well as $\gamma_1^{(1)} = -\bar{\mu}_1$, $\gamma_2^{(1)} = 0$, $\theta_1^{(1)} = \theta_2^{(1)} = 1/2$, $\eta_1^{(1)} = -\eta_2^{(1)} = -\bar{\mu}_1$ in Eqs. 24 and 25. Fig. 2 shows $y_1(x, t)$ for $M = 10^4$ and $N_1 = 10^2$ at five different times, from the initial distribution at $t = 0$ (marked t_1) to equilibrium $t \rightarrow \infty$ (marked t_5). The two initially separated distributions, a delta-peak at $x = 0$ and a pre-equilibrated Gaussian at $x = 200$, move together and merge into a single Gaussian that represents equilibrium. The inset shows $y_1(x, t)$ for the same system and time sequence yet subject to the starting distribution of a boxcar function located at $x = 100 \pm 70$.

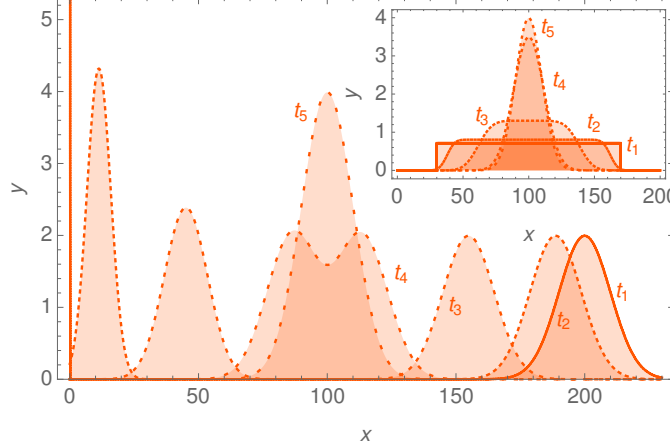


FIG. 2: 50 empty NCs are added to 50 pre-equilibrated NCs (all of the same type, $L = 1$) that contain 10,000 cargo items, implying $M = 10^4$ and $N_1 = 10^2$ and thus $\bar{\mu}_1 = M/N_1 = 100$. Distributions $y_1(x, t)$ are displayed at various times (all measured in units of ζ_1): $t_1 = 0$, $t_2 = 0.12$, $t_3 = 0.6$, $t_4 = 2$, $t_5 \rightarrow \infty$. The delta-peak at $x = 0$ corresponds to the initially empty NCs and thus encloses an area $N_1/2$. The inset shows $y_1(x, t)$ for the same time sequence subject to the starting distribution of a boxcar function located at $x = 100 \pm 70$.

In the presence of two distinct NC types ($L = 2$), the rate matrix $\{\{-K_{12}N_2, K_{21}N_1\}, \{K_{12}N_2, -K_{21}N_1\}\}$ has the eigenvalues $\lambda_1 = -K_{eff}$ with $K_{eff} = K_{12}N_2 + K_{21}N_1$ and $\lambda_2 = 0$ as well as eigenvectors $-b_{11} = b_{21} = b_{22} = 1$ and $b_{12} = \kappa/(1 - \kappa)$ with $\kappa = K_{21}N_1/K_{eff}$. Demanding a fraction η of the M cargo items initially in component 1 specifies $c_1 = -M(\eta - \kappa)$ and $c_2 = M(1 - \kappa)$, implying $M_1(t)/M = \kappa + e^{-K_{eff}t}(\eta - \kappa)$ and $M_2(t)/M = 1 - \kappa - e^{-K_{eff}t}(\eta - \kappa)$. Following the calculation of W_{ln} , $P_l(t)$ and $Q_l(t)$, the functions $y_1(x, t)$ and $y_2(x, t)$ are only subject to specifying the initial distributions $f_1(x)$ and $f_2(x)$. Fig. 3 shows an example for $\eta = 0.15$, with initially a Gaussian distribution for $f_1(x)$ (shown in orange) and a boxcar function for $f_2(x)$ (shown in purple).

The presence of many NC types requires, in general, the eigenvalues and corresponding eigenvectors of the rate matrix to be calculated numerically. Following that, Eq. 17, 21, or 24 immediately provide access to all distributions $y_l(x, t)$. Fig. 4 shows an example for $L = 4$ (color-coded as in Fig. 1), where initial distributions consisting of single Gaussians for components 1 (orange) and 3 (yellow) and a superposition of two Gaussians for components 2 (purple) and 4 (green) evolve toward their equilibrium. The insets show the total numbers

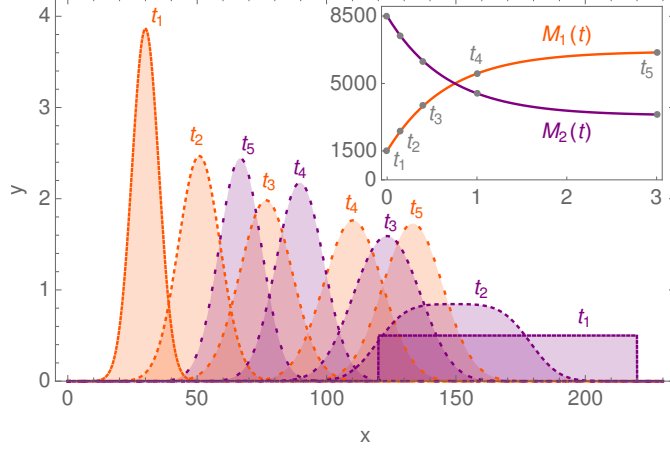


FIG. 3: $N_1 = 50$ type-1 NCs (acceptors) and $N_2 = 50$ type-2 NCs (donors) initially carry 1500 and 8500 cargo items, respectively. The selected rate constants $K_{11} = 2$, $K_{12} = 1$, $K_{21} = 2$, $K_{22} = 5$ (all measured per inverse time unit) yield $K_{eff} = 150$ and $\kappa = 2/3$, implying that type-1 NCs will hold 67% of the cargo items after a long time. The Gaussians at equilibrium, $t \rightarrow \infty$ (marked by t_5), are located at $\bar{\mu}_1 = 133.3$ and $\bar{\mu}_2 = 66.7$. At $t = 0$ (marked by t_1) the system starts from a single Gaussian (with $\gamma_1^{(1)} = -0.8 \bar{\mu}_1$) for the acceptors and a boxcar function located at $x = 170 \pm 50$ for the donors. Distributions $y_1(x, t)$ (orange) and $y_2(x, t)$ (purple) are shown at five different times: $t_1 = 0$, $t_2 = 0.15$, $t_3 = 0.4$, $t_4 = 1$, $t_5 \rightarrow \infty$, all measured in units of K_{eff}^{-1}/N . These times are marked by gray bullets in the inset, which shows the time evolutions $M_1(t)$ and $M_2(t)$ of cargo in acceptors and donors.

of cargo items $M_l(t)$ and the second moments $S_l(t) = \int_{-\infty}^{\infty} dx (x - M_l(t)/N_l)^2 y_l(x, t)$ in l -type NCs. The second moment characterizes how the width of the distribution evolves over time.

In summary, analyzing the transfer kinetics of cargo in ensembles of mobile NCs with distinct chemical identities yields analytic solutions in the Gaussian regime, subject to assuming all cargo items are independent and randomly distributed among the available identical sites. This work advances the use of chemical reaction kinetics for the modeling of cargo transfer in multicomponent systems, with possible extensions to account for cargo aggregation inside the carriers, spatial resolution of transfer processes, and non-identical nanocarrier sites.

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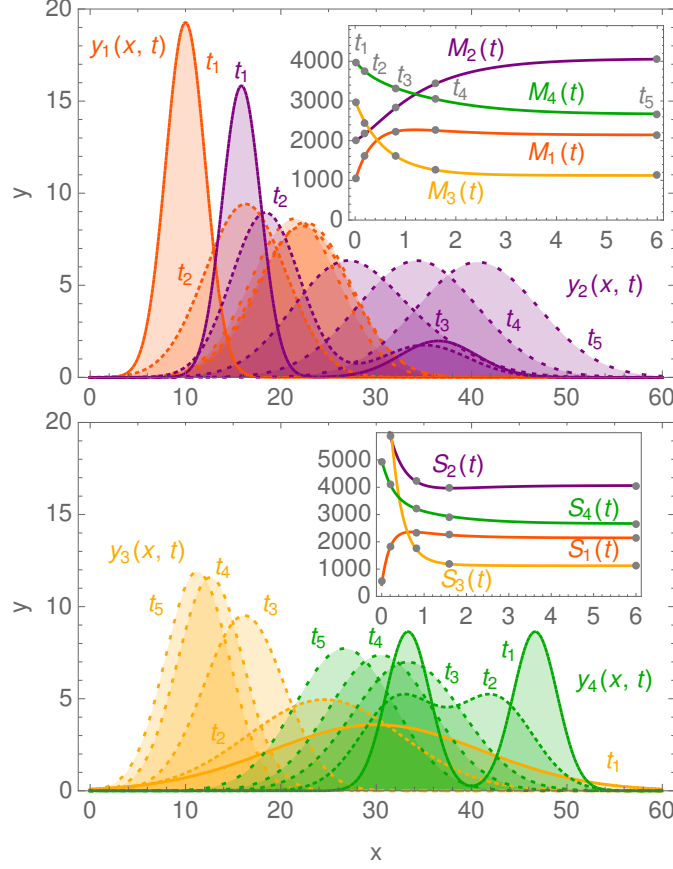


FIG. 4: A system containing four distinct NC types (displayed in orange, purple, yellow, green – matching the color scheme in Fig. 1), each present with 100 NCs that carry initially normal distributed $i \times 10^3$ cargo items ($i = 1, 2, 3, 4$). Rate constants are randomly selected, $K_{kl} = 10^{-3} \times \{\{4.6, 9.1, 2.9, 8.3\}, \{3.6, 4.5, 1.6, 0.85\}, \{8.9, 1.3, 4.2, 4.5\}, \{7.0, 1.4, 1.5, 4.4\}\}$. Distributions $y_l(x, t)$ are displayed at five times t_i , starting from $t_1 = 0$ to t_5 near equilibrium. These times are marked by gray bullets in the insets, which show the time evolution of the total number of cargo items $M_l(t)$ (upper inset) and the second moment $S_l(t)$ (lower inset) in type l -NCs.

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