

The discrete puff model

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Discrete model

The discrete model consists of a lattice of length L . The dynamics is controlled by a set of parameters

ω_s	the puff splitting rate
ω_d	the puff decay rate
p	the puff hopping rate
λ_{push}	pushing length-scale
q_{sup}	suppression parameter for puffs within a distance λ_{push}
q_{push}	pushing parameter for puffs within a distance λ_{push}

In the basic version of the model, particles hop to the right with a probability p in each time step. We permit puff suppression by allowing a right hopping particle to invade an occupied neighboring site and thereby eliminate a downstream puff/particle. Note that we have also considered a variant of the model where we do not permit puff suppression, meaning that particles do not hop if it results in a collision with an already occupied site. The lifetime $\tau_{d,\infty}$ and time between splitting events, $\tau_{s,\infty}$, are given by the empirical functions

$$\tau_{d,\infty}(\text{Re}) = \exp(\exp[0.005898 \text{ Re} - 9.1871]),$$

The corresponding expression for the splitting rate is given by

$$\tau_{s,\infty}(\text{Re}) = \exp(\exp[-0.003165 \text{ Re} + 9.2871]).$$

The model is performed using one of two update rules, an upstream update rule, where the puffs in each time step are updated sequentially from the left to the right and a stochastic update rule (producing similar results (in almost all circumstances)) where puffs are picked randomly one-by-one and updated accordingly.

The dimensionless diffusion constant D of the right hopping process is

$$\tilde{D} = \frac{p(1-p)}{2}$$

Puff-pushing and suppression

The puff-pushing alters the hopping probability p of a puff x_i depending on the distance $|x_i - x_{i-1}|$ to an upstream puff x_{i-1} . If that distance is smaller than some pushing length λ_{push} , the hopping probability is set to one, i.e.

$$\text{hopping probability of puff at } x_i = \begin{cases} p & \text{if } |x_i - x_{i-1}| > \lambda_{push} \\ q_{push} = 1 & \text{if } |x_i - x_{i-1}| \leq \lambda_{push} \end{cases}$$

We use the following expression for the probability of puff-suppression, when a puff is within a distance $d < d_{sup}$ from an upstream puff

$$\text{Suppression probability of a puff at } x_i = \begin{cases} 0 & \text{if } |x_i - x_{i-1}| > \lambda_{push} \\ q_{sup} & \text{if } |x_i - x_{i-1}| \leq \lambda_{push} \end{cases}$$

Comparison to experimental values

The experiments have the following characteristic parameters

D^*	4e-3 m
U^*	0.4995 ms ⁻¹
L^*	6.3e-5 m ² s ⁻¹
T^*	8e-3s = $(D^*)/(U^*)$

In the experiments, a puff has a spatial extent of $\lambda = 12D^*$. For a pipe of length $7800D$ and with a pushing zone reaching out to $\lambda_{push} = 4\lambda$, a system being in the perfect puff-crystal state would contain around $7800/48 = 162$ puffs. If we convert these numbers to units of the discrete model, the corresponding system size would be $162\lambda_{push}/\lambda$ lattice units. We can perform meaningful simulations down to values of $\lambda_{push} = 2\lambda$ i.e. a discrete system representing the experimental system would consist of around 350 lattice units.

Regardless of the model, the scaling of the dimensionless variables should result in the same variables with dimensions, e.g.

$$L^* = \frac{p(1-p)}{2} \frac{\lambda^2}{\tau} \quad (1)$$

Here λ is a characteristic length scale and τ a characteristic time scale for the model.

All the relevant timescales in the model are scaled with this length and time, where e.g. dimensionless reaction rates become

$$\begin{aligned} \omega_{\text{decay}}(\text{Re}) &= \frac{\tau}{\tau_{d,\infty}(\text{Re})} \\ \omega_{\text{split}}(\text{Re}) &= \frac{\tau}{\tau_{s,\infty}(\text{Re})} \end{aligned}$$

The scale parameters are determined by matching the model to the characteristics of the experiment. First we choose our length scale to be as large as possible without losing the microscopic details, e.g. the length scale should be smaller than the pushing distance such that puff-pushing is resolved. Here we choose

$$\lambda = 12 D^*,$$

i.e. the spatial extent of a puff. We choose $p = 0.5$ and therefore our timescale follows from Eq. (1),

$$\tau = \frac{p(1-p)}{2} \frac{\lambda^2}{L^*}. \quad (2)$$

Note that it is computationally advantageous to use as large as possible a diffusion constant, which would mean $p = 0.5$.

Code

The code used to simulate the discrete model is included as a subroutine in the `c++` file with the name

`puff_pushx.cpp`

The subroutine can be called from a simple script file using the statistical language R. In the script, the different parameters of the model can be set.

`puff_beta_runx.R`