A one-dimensional modified TASEP model on a track of variable length: analytical and computational results

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Abstract. We present analytical solutions and Monte Carlo simulation results for a one-dimensional modified TASEP model inspired by the interplay between molecular motors and their cellular tracks of variable lengths, known as microtubules. Our TASEP model incorporates rules for changes in the length of the track based on the occupation of the first two sites. Using mean-field theory, we derive analytical results for the particle densities and particle currents and compare them with Monte Carlo simulations. These results show the limited range of mean-field methods for models with localized high correlation between particles. The variability in length adds to the complexity of the model, leading to emergent features for the evolution of particle densities and particle currents compared to the traditional TASEP model.

1. Introduction

Traffic models have been of interest to physicists and mathematicians for a very long time for their versatile interdisciplinary applications. For biophysicists, it is interesting to study how traffic jams at the intracellular level may affect the proper functioning of the cell. Stochastic processes driving traffic jam formation appear in many physical systems and have been thoroughly studied in physics, chemistry, biology and social sciences using a variety of stochastic models. One category of models that lead to useful quantitative results for different traffic-type models is the totally asymmetric exclusion process (TASEP), studied by itself to isolate edge effects in smaller systems [1] or coupled with Langmuir kinetics to model bulk dynamics [2, 3].

We discuss in this paper the TASEP special case of a more general model presented by our group in [4] and based on previous studies such as [5, 6, 7, 8]. The general model is amenable to Monte Carlo simulations but it is too complex to lead to meaningful analytical results. The version of the model focused on TASEP can be easily adapted to other TASEP-type traffic systems from biology or elsewhere. In section 2, we introduce our TASEP model and present the relevant mean-field equations. In section 3 we discuss the main results. We present further work and possible applications in section 4.
2. Model rules and mean-field dynamics

Our model is a special case of the model presented in [4]. For convenience, we summarize it here but we invite the reader to consult [4] for further details. The model is defined on a one-dimensional lattice of variable length with $N$ sites, representing the microtubule. Each site can be empty or occupied by a particle (the representation of our molecular motor) represented by an occupation number $n_i = 0$ for empty and $n_i = 1$ for occupied. The right end is fixed (site $N$), and the left end (site 1) can extend, remain the same or contract. Following the same method as in [5, 6], we choose a reference frame attached to the growing tip of the filament, with site 1 being the leftmost site. Any site “i” measures the distance of that site from the fluctuating tip. When the lattice grows or shrinks due to the attachment or detachment of a new site at the tip, respectively, all the site labels are updated $i ightarrow i \pm 1$. The particle traffic flows from right to left.

The special case of the general model does not include the attachment and detachment of particles along the track, as in Langmuir dynamics. Rather, this scenario allows only for the entrance and exit of particles at the terminal sites of the track. The system evolves according to the following rules (as presented in in Fig. 1):

At sites 1 and 2:

- $10 \rightarrow 00$ with rate $\beta$: particles leave the track with exit rate $\beta$;
- $01 \rightarrow 10$ with rate 1: particles move from right to left if the neighboring site is empty;
- $00 \rightarrow 000$ with rate $\gamma$: the length of the track increases by one unit when the two first sites are empty; this is equivalent to spontaneous polymerization of a microtubule;
- $11 \rightarrow 0$ with rate $\delta$: the length of the track decreases by one unit when two particles (occupying site 1 and 2) are present, at the same time, the particles leaves the track; this is equivalent to motor-induced depolymerization for a microtubule;

In bulk (sites $n_i = 3...N-1$):

- $01 \rightarrow 10$ with rate 1: particles move to the left with rate 1 as long as the neighbor to the left is empty;

At site $N$:

- $00 \rightarrow 01$ with rate $\alpha$: particles enter the track with entrance rate $\alpha$;
- $01 \rightarrow 10$ with rate 1: diffusion to the left with rate 1.

We present below the evolution equations for the site occupation numbers. Further details about the derivation of the equations can be found in [4]:
\[ \frac{dn_1}{dt} = -\beta n_1(1 - n_2) + n_2(1 - n_1) - \delta n_1 n_2 \]

\[ \frac{dn_2}{dt} = n_3(1 - n_2) - n_2(1 - n_1) - \delta n_1 n_2 n_3 + \delta n_3 n_2 n_3 \]

\[ \frac{dn_3}{dt} = n_4(1 - n_3) - n_3(1 - n_2) - \gamma(1 - n_1)(1 - n_2) n_3 + \delta n_1 n_2 (n_4 - n_3) \]

\[ \frac{dn_4}{dt} = n_{i+1}(1 - n_i) - n_i(1 - n_{i+1}) + \gamma(1 - n_1)(1 - n_2)(n_{i-1} - n_i) + \delta n_1 n_2 (n_{i+1} - n_i), \text{ for } n_i = 4 \ldots N - 1 \]

\[ \frac{dn_N}{dt} = \alpha (1 - n_N) - n_N (1 - n_{N-1}) \]

We define the the mean local densities as the mean ensemble values of the site occupation numbers \( \rho_i = < n_i > \) and we replace the mean correlations between site occupation numbers with the product of their averages: \( < n_i n_j > = \rho_i \rho_j \). With these assumptions in mind, the equations above become:
\[
\begin{align*}
\frac{d\rho_1}{dt} &= -\beta \rho_1 (1 - \rho_2) + \rho_2 (1 - \rho_1) - \delta \rho_1 \rho_2 \\
\frac{d\rho_2}{dt} &= \rho_3 (1 - \rho_2) - \rho_2 (1 - \rho_1) - \delta \rho_1 \rho_2 + \gamma \\
\frac{d\rho_i}{dt} &= \rho_{i+1} (1 - \rho_i) - \rho_i (1 - \rho_{i-1}) + \gamma (1 - \rho_i) (1 - \rho_2) (\rho_{i-1} - \rho_i) + \delta \rho_1 \rho_2 (\rho_{i+1} - \rho_i), \text{ for } n_i = 4 \ldots N - 1 \\
\frac{d\rho_N}{dt} &= \alpha (1 - \rho_N) - \rho_N (1 - \rho_{N-1}) 
\end{align*}
\]

Following the same method as in [4, 9, 2], the continuous equation for the bulk density \((n_i = 4 \ldots N - 1)\) for the steady-state is:

\[
(C - 2\rho(x)) \left( \frac{d\rho(x)}{dx} \right) = 0
\]

where \(C = \gamma (1 - \rho_2) (\rho_1 - 1) + \delta \rho_1 \rho_2 + 1\).

This equation can be rewritten as a continuity equation:

\[
\frac{dJ(x)}{dx} = 0
\]

where the particle current is defined as \(J(x) = \rho (C - \rho)\).

The continuous version of the evolution equation for the fixed tip (re-scaled as \(x = 1\) with the approximation \(N - 1 \approx N\) in the thermodynamic limit) is:

\[
\frac{d\rho(1)}{dt} = (\alpha - \rho(1)) (1 - \rho(1))
\]

3. Analytical and computational results

For the TASEP model presented here, one end of the track is fixed, while the other one can undergo growth or shrinkage. Track growth and shrinkage are dictated by the presence or absence of dimeric protein subunits, called alpha-beta tubulin, consistent with the biological literature on polymerization and depolymerization of microtubules [10].

The solution for the density is not dependent on \(x\); it is a constant that incorporates the densities of boundary sites 1 and 2. Specifically, the bulk solutions for the steady state particle density and current are equal to:

\[
\rho(x) = \frac{C}{2} = \frac{(1 - \rho_2) (\rho_1 - 1) + \delta \rho_1 \rho_2 + 1}{2}
\]

\[
J(x) = \rho (C - \rho) = \frac{C^2}{4} = \frac{(1 - \rho_2) (\rho_1 - 1) + \delta \rho_1 \rho_2 + 1}{4}
\]

If the length is constant \((\gamma = 0 \text{ and } \delta = 0)\), we recover the well-known TASEP result of a bulk density equal to 0.5 and a constant current of 0.25 for the maximum current phase, as
reported in [9]. For the right boundary, the constant of integration is equal to \( \alpha \), the entrance rate, as derived from Eq. 5 for the steady state. For the left boundary, the density is equal to \( \rho_3 \), considered as our boundary site. Given the high correlation between sites 1 and 2, they can be seen, intuitively, as one unit, a “dimer”.

To summarize, the density profile is a piece-wise function as follows:

\[
\rho(x) = \begin{cases} 
\rho_3 & \text{at the left boundary (position of the moving tip)} \\
\frac{\gamma(1-\rho_2)(\rho_1-1)+\beta\rho_2+1}{2} & \text{in the bulk} \\
\alpha & \text{at the fixed right boundary}
\end{cases}
\]

(7)

And for the steady-state current:

\[
J(x) = \begin{cases} 
\rho_3(C - \rho_3) & \text{at the left boundary (position of the moving tip)} \\
\frac{\gamma(1-\rho_2)(\rho_1-1)+\beta\rho_2+1}{2} & \text{in the bulk} \\
\alpha(C - \alpha) & \text{at the fixed right boundary}
\end{cases}
\]

(8)

The discussion of density and current profiles in the parameter space becomes exceedingly complex with so many parameters in play. For specific sets of parameters, we can find the numerical values for densities \( \rho_1, \rho_2 \) and \( \rho_3 \), which in return lead to numerical values for the steady-state bulk densities and currents. We present some special cases in the hope that they will lead to a more profound and intuitive understanding of the complexities of this model and may be used as templates for practical applications in modeling traffic at the cellular level.

3.1. \( \delta = 0 \)

The first case that we discuss is \( \delta = 0 \) (no shrinkage allowed when the first two sites are occupied). This describes a microtubule in the growth (polymerization) phase for which a cap of motors at the moving tip doesn’t trigger a shortening of the microtubule, a phenomenon known in the literature as “microtubule catastrophe” [11]. In this situation, the mean-field solutions for the first three site densities have more manageable expressions obtained by solving Eq. 3 for the case \( \delta = 0 \):

\[
\begin{align*}
\rho_1 &= \frac{\gamma - \sqrt{\beta\gamma(1-\beta)}}{\beta^2 - \beta + \gamma} \\
\rho_2 &= \frac{\beta\rho_1}{1-\rho_1(1-\beta)} \\
\rho_3 &= \beta\rho_1
\end{align*}
\]

(9)

It is interesting to see that if \( \gamma = 0 \) as well (no polymerization allowed), we recover again the well-known TASEP result of a bulk density equal to 0.5 and a constant current of 0.25 for the classical TASEP maximum current phase [9], regardless of the values of \( \alpha \) and \( \beta \). However, from the equations above we can see that if \( \gamma = 0, \rho_1 = \rho_2 = \rho_3 = 0 \). So we have a cap of three empty sites followed by a jump in density to 0.5, and the fixed end will be at a density dictated by the entrance rate \( \alpha \).
The Monte Carlo simulations tell a different story, as presented in Fig. 2. Due to the strong correlations between the first two sites at the moving tip, particles leave the track only when the first site is occupied and the second site is empty, and they are forbidden to leave (due to $\delta = 0$) when both sites are occupied. Therefore, the steady-state density is close to 1 even in the case of $\beta > \alpha$, which is different from the classic TASEP model result.

This strong correlation is not captured in the mean-field equations, and it leads to drastically different results. The bulk density is constant for $\alpha \geq \beta$, but it settles at almost double the mean-field value. The track is almost full, which leads to a small current along the track. For $\alpha < \beta$, the average site density has a linear dependence on the position, with a corresponding decreasing current. In the time-dependent graphs presented in Fig. 2d, we notice the interesting feature of a maximum in current, with the peak shifted to the right for $\alpha < \beta$.

Another interesting case worth mentioning for the growing regime ($\delta = 0$, $\gamma \neq 0$) is the case of $\beta = \gamma$, for which the first three densities simplify to:

$$
\rho_1 = \frac{1 - \sqrt{1 - \beta}}{\beta} \quad \rho_2 = \frac{\beta (\sqrt{1 - \beta} - 1)}{(\beta - 1) \sqrt{1 - \beta} - 2\beta + 1} \quad \rho_3 = 1 - \sqrt{1 - \beta}
$$

When $\beta = \gamma \rightarrow 1$, the tip has a cap of densities $\rho_1 = \rho_2 = \rho_3 = 1$ and the bulk density settles at 0.5. When $\beta = \gamma \rightarrow 0$, $\rho_2 = \rho_3 = 0$ but $\rho_1 = 0.5$, leading to a bulk density of again 0.5. The dependence of the bulk density and the bulk current on $\beta$ in comparison with the Monte Carlo simulations are presented in Fig. 3. As we can see from the graphs, contrasted with the simplicity of the mean-field solutions, the Monte Carlo simulations show a more complex behavior of the system that merits a more in-depth analysis. The mean-field solutions are somewhat close to the simulations results for a very small interval around $\beta = \gamma = 0.3$.

In Fig. 4 we present sample Monte Carlo data for the polymerization case ($\delta = 0$ and $\beta \neq \gamma$). Again, we have a discrepancy between the mean-field theory and the simulations. The qualitative solution of constant bulk density is captured by MC simulations for values of $\beta > \gamma$, where the density is constant between $x \in (0, 0.15)$ and then it drops to 0. Although for the small interval of $x$ the density is constant in MC simulations, the value is twice the mean-field value of 0.42. The corresponding MC current has a peak of 0.125, close to the mean-field value of 0.17. For $\beta \leq \gamma$ the MC bulk density displays a linear decrease along the track. The mean-field solution for the density does not capture this decrease, as it is a constant equal to 0.48. The MC current is close to the mean-field solution of 0.23 for $x \in (0, 0.1)$.

### 3.2. $\gamma = 0$

The other limit case is $\gamma = 0$, for which the track can only shrink when the two sites at the tip are occupied. This describes the motor-induced depolymerization for a microtubule [12].
Figure 2: The case of constant length tracks: (a) average steady-state site density along the track; (b) average steady-state current along the track; (c) the time evolution of the total density; (d) the time evolution of the total current.

In this case, the expressions for $\rho_1$, $\rho_2$ and $\rho_3$ are:

$$\rho_1 = \frac{\beta + \delta - 1}{\delta + \beta - 1}$$  \hspace{1cm} (11)$$

$$\rho_2 = \rho_3 = \frac{\beta - 1}{\beta}$$  \hspace{1cm} (12)$$

and they are confined to $\beta + \delta < 1$ to maintain their values between zero and 1.

It is interesting to see that if we set $\delta = 0$, the first three sites have a density equal to one. In the previous case, when we started with the solution for $\delta = 0$ and then turned off $\gamma$ as well,
Figure 3: Special case of polymerization regime: Comparison between mean-field and the MC results for bulk densities (a) and currents (b) as functions of $\beta = \gamma$, with $\alpha = 0.5$.

Figure 4: Monte Carlo results for the polymerization regime $\delta = 0$, $\alpha = 0.5$, and initial length $N = 100$: (a) average density along the track; (b) average current along the track.

the cap was all empty sites. Overall, when the track is not allowed to shrink or expand, $\rho_1$, $\rho_2$, $\rho_3$ are all 0 or 1, forming a cap of empty sites that will tend to polymerize or a cap of full sites that will trigger depolymerization.

Fig. 5 shows the average site density and the current density along the track, as well as the total density and current for two cases of $\beta < \delta$ and $\beta > \delta$. The mean-field theory predicts a constant bulk density and current for a given set of parameters. A qualitative agreement holds for the current in the case of $\beta = 0.8$, $\delta = 0.1$ for a small portion of the track $x \in (0, 0.04)$, with $J_{MC} = 0.25$ and $J_{MF} = 0.267$ (a 6.8% difference). The densities compare well for the beginning of the track: 3.4% difference for $\beta = 0.8$, $\delta = 0.1$, but the trend shown in Monte Carlo simulations is not the one predicted by the mean-field theory. For the $\beta = 0.1$, $\delta = 0.8$ case, the system doesn’t reach a steady-state. It is interesting to see the unusual behavior of the total.
density and total current as functions of time. From the plots, we can identify the position of the domain walls where the current suddenly drops to a lower value, then continues to decrease linearly, signaling the presence of traffic jams. Because there is no steady-state, Fig. 5 (a) and Fig. 5 (b) represent the average site density and average site current along the track after the system underwent a set number of Monte Carlo steps. It is a snapshot of the system, but not its steady-state. These unusual features deserve a further systematic investigation in future studies.

![Graphs showing Monte Carlo results for the depolymerization regime γ = 0 and initial length N = 100: (a) average site density along the track; (b) average site current along the track; (c) the time evolution of the total density; (d) the time evolution of the total current.](image)
3.3. $\gamma \neq \delta \neq 0$

We now present a sample set of data for the case of $\gamma \neq \delta \neq 0$, $\alpha = 0.8$, $\beta = 0.1$, $\gamma = 0.07$ and $\delta = 0.95$ and an initial number of 100 sites and a maximum number of 500 sites (Fig. 6). This sample case captures the switch between growth and shrinkage for the microtubules, known in literature [11] as microtubule instability. For the Monte Carlo simulations we ran a whole range of track sizes, from 100 to 5000 initial number of sites. The main results remain qualitatively the same.

The mean field predicts in this case a bulk density of $\rho = \frac{1-\gamma}{1+\gamma}$, the Monte Carlo simulations give us a value of approximately 0.46, and the mean-field current has a value of 0.25. Although the mean-field results for the bulk density and current seem to agree with the simulations, this comparison doesn’t take into account the time scale of the track length fluctuations and the time it takes for the system to reach steady state. In our model they are on the same order. If the time scale of the track length fluctuations were much smaller than the time needed to reach steady state, one may consider the track to be of essentially constant length.

4. Conclusions

We discussed in detail, using mean-field techniques and Monte Carlo simulations, a TASEP traffic model defined on variable tracks in the context of motion of molecular motors on microtubules. Although the mean-field theory is limited in use for this model, we were able to derive analytical results that capture qualitatively the microtubule instability and the clustering of particles at the microtubule end for specific sets of parameters. The model can be refined to include entrance and exit rates that are particle density dependent or time dependent. As mentioned in [4], another avenue of study may be a kinetic approach to small-size systems by solving numerically the governing master equation.

TASEP-type models are also useful in modeling translation, the process in which transfer RNAs convert messenger RNA transcripts into a polypeptide chain [13]. The model can also be generalized to multiple, parallel tracks with entrance and exit rates, which would be a more realistic representation of molecular motors traffic.

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Figure 6: Microtubule instability. Monte Carlo results for the case of $\gamma \neq \delta \neq 0$ and initial length $N = 100$ and maximum number of 500 sites, $\alpha = 0.8$, $\beta = 0.1$, $\gamma = 0.07$ and $\delta = 0.95$: (a) average density along the track; (b) average current along the track; (c) the time evolution of the total density; (d) the time evolution of the total current; (e) The average length of the microtubule as a function of time.