

Supporting Information

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SI Text

Simulation Details. The Brownian dynamics simulations are performed in a 2D box of size $L \times L$ with periodic boundary conditions. The box is decorated randomly with annular domains (taken from a uniform distribution with density, ρ_a) whose inner and outer radii are r_c and R , respectively. These annular domains contain a uniform concentration c_0 of polar filaments pointing radially inward. In between the domains the polar filaments are distributed randomly in space and orientation. The annular domains represent the inward pointing asters, whose size is R and $r_c \ll R$, the core size. When particles (molecules) enter these domains, they are advected toward the core of the asters with a velocity, v . The aster domains dynamically remodel—they break up and reform at a random location within the simulation box, in a time taken from an exponential distribution with a mean remodeling time given by τ_a .

On this dynamical background, we sprinkle a low concentration of the reactant molecules. For example, we may start with a low concentration of A molecules ($N = 100$) distributed randomly in the 2D box. A few of these molecules $N_{A^*} = 10$ are taken to be in conformation A^* at time $t = 0$. The molecules can stochastically bind and unbind onto the filaments, with rates k_{on} and k_{off} , respectively; in the bound state the molecules are advected along the polar filament with velocity v , whereas in the unbound state the molecules diffuse in the 2D plane with an effective diffusion coefficient D .

All lengths are measured in units of σ (the size of molecule (particle) A), and time is set by the diffusion time $\tau_d = \sigma^2/D$ over this scale. The simulation proceeds in steps of $\Delta t = 0.1\tau_d$. The dimensionless parameters in the simulation are $\tau_a = 10$ – 10^5 , advection time $\tau_v = 0.1$ – 10^4 , $r_c = 2$, and $R = 100$. The size of the box is set to $L = 1,000$ unless otherwise stated. The mean duty ratio, $K = k_{\text{on}}/(k_{\text{on}} + k_{\text{off}})$, varies between 0.5 and 1.

Thus, for instance, if we choose $\sigma = 10^{-9}$ m and $D = 1.0 \mu\text{m}^2/\text{s}$, then we get for the unit of time, $\tau_d = \sigma^2/D = 1 \mu\text{s}$. On the other hand, if we choose $\sigma = 10^{-8}$ m and $D = 0.1 \mu\text{m}^2/\text{s}$, we get a $\tau_d = 1$ ms.

At every time step, a molecule depending upon its state does the following:

Diffusion. If a molecule (A or A^*) is outside the aster domains, then it diffuses with an effective diffusion coefficient, D . In this case, the positions of the molecule are updated according to

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \Delta \mathbf{r}, \quad [\text{S1}]$$

where each component Δr_α ($\alpha = 1, 2$) is chosen independently from a Gaussian distribution with zero mean and variance given by $\langle (\Delta r_\alpha)^2 \rangle = 2D\Delta t$.

Advection. If a molecule (A or A^*) is bound to one of the aster domains, then it moves radially inward toward the core of the aster. The position updates for advection happen according to

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}\Delta t. \quad [\text{S2}]$$

Note that during advection, a bound molecule may become unbound with a rate k_{off} , in which case they would diffuse according to Eq. S1.

Reaction. If A and A^* come within a distance of r_c (either within or out of the domain), then they either react with a rate k_f (forward reaction),



or react with a rate k_b (backward reaction),



In case the reaction is irreversible only Eq. S3 is performed. Because the reaction range has been taken to be of order of the aster core size, the aster cores become active reaction zones.

Defining $M(t) = N_{A^*}(t)/N$, the instantaneous fraction of A^* , we can compute the mean activation time τ and the saturation output, M_∞ . Note that for the irreversible dynamics, $M_\infty = 1$. To compare our results with free diffusion, we performed simulations with the same system without the aster domains. In this case we have both reaction and diffusion but no advection. We can then plot the gain in the activation rate defined as $G_\tau = \tau_{\text{diff}}/\tau_{\text{act}}$, where τ_{diff} and τ_{act} are the mean activation times for free diffusion and active dynamics, respectively, against various dynamical parameters. Note that in our simulations, we average over at least 100 initial conditions.