Table 1: Parameter specs for different simulation techniques. .

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Volume  (μm3) | Surface Area  (μm2) | (μM) | (μM) | (μm-2) | (M-1) | (M-1) | koff  (s-1) | (M-1 s-1) | (M-1 s-1) |
| FPR | 0.166 | 0.218 | 1 | 1 | 17000 | 107 | 2 106 | 1 | 107 | 2 106 |
| ODE-Mathematica | 50 | 65.63 | 1 | 1 | 17000 | 107 | 2 106 | 1 | 107 | 2 106 |
| ODE-VCell | 50 | 65.63 | 1 | 1 | 17000 | 107 | 2 106 | 1 | 107 | 2 106 |
| SSA-VCell | 50 | 65.63 | 1 | 1 | 17000 | 107 | 2 106 | 1 | 107 | 2 106 |
| PDE-VCell | 50 | 65.63 | 1 | 1 | 17000 | 107 | 2 106 | 1 | 107 | 2 106 |
| Smoldyn-VCell | 0.166 | 0.218 | 1 | 1 | 17000 | 107 | 2 106 | 1 | 107 | 2 106 |
| Theory | 50 | 65.63 | 1 | 1 | 17000 | 107 | 2 106 | 1 | 107 | 2 106 |

Table **S4g** Equilibrium concentrations of species in Network{M,P1,P2} with specs shown on Table 1. Mean and standard deviations () in parentheses provided for stochastic simulations.10 SSA trajectories taken. For PDE, spherical geometry simulated (Mesh:31x31x31) with maximum timestep 0.001s. Smoldyn (Mesh:27x27x57) has the same reaction geometry as the FPR and timestep is 1μs. 8 Smoldyn trajectories.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Equilibrium  Concentrations | (M-1) | (μM) | (μM) | (μM) | (μM) | (μM) | (μM) | (μM) | (μm-2) |
| FPR  (24 Traj) | 4.072 109  (3.902 109) | 0.9846  (0.0078) | 0.0062  (0.0049) | 0.0154  (0.0078) | 0.0154  (0.0078) | 0  (0) | 0  (0) | 0.0004 (0.002) | 16082.07  (0) |
| ODE-Mathematica | 3.691 109 | 0.9836 | 7.3662 10-5 | 0.0161 | 0.0161 | 5.2529 10-7 | 2.2581 10-4 | 2.2581 10-4 | 16089.15 |
| ODE-  VCell | 3.688 109 | 0.9833 | 7.3636 10-5 | 0.0161 | 0.0161 | 5.2513 10-7 | 2.2916 10-4 | 2.2916 10-4 | 16082.98 |
| SSA-  VCell (10) | 3.799 109 | 0.9835  (0.0004) | 4.6496 10-5  (5.4684 10-5) | 0.0159  (3.429 10-4) | 0.0159  (3.429 10-4) | 3.3223 10-6  (1.0506 10-5) | 2.2924 10-4  (8.0629 10-5) | 1.5282 10-4  (5.980110-5) | 16082.95  (0.0613) |
| PDE-VCell | 3.709 109 | 0.9889 | 7.4081 10-5 | 0.0161 | 0.0161 | 5.2848 10-7 | 2.2989 10-4 | 2.2989 10-4 | 16077.77 |
| Smoldyn-  VCell (8) | 7.843 109 | 0.9650  (0.0107) | 0  (0) | 0.0350  (0.0107) | 0.0338  (0.0119) | 0  (0) | 0.0014  (0.0035) | 0  (0) | 16081.26  (1.6059) |
| Theory | 3.703 109 | 0.9835 | 7.4747 10-5 | 0.0162 | 0.0162 | 5.3307 10-7 | 2.3088 10-4 | 2.3088 10-4 | 16082.68 |