Supplementary Information
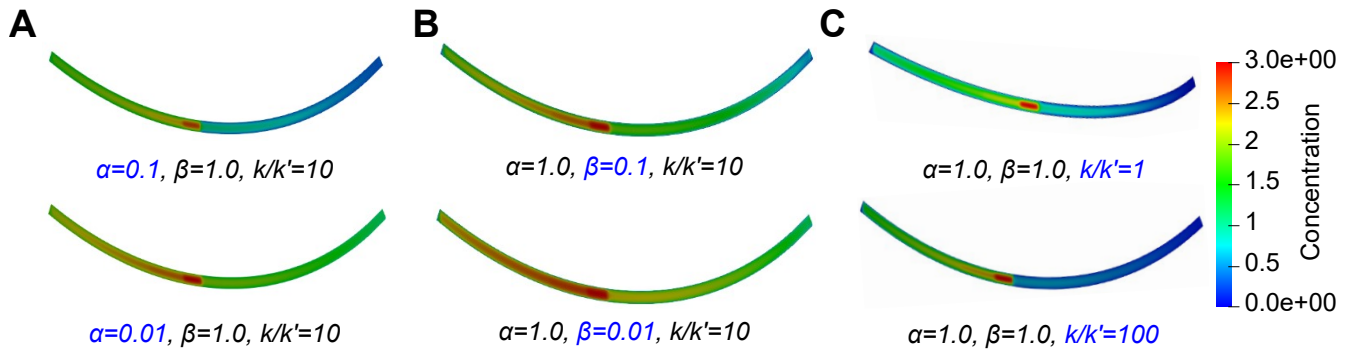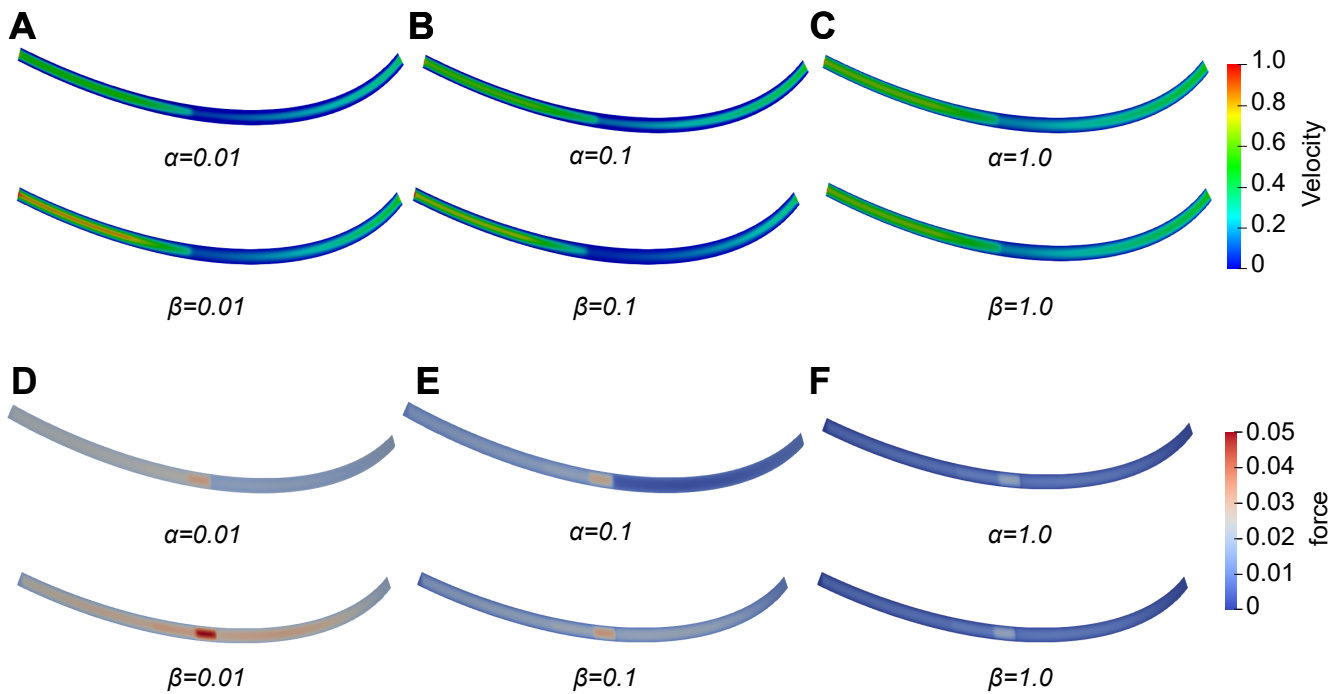# Modeling material transport regulation and traffic jam in neurons using PDE-constrained optimization

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Supplementary Figures

A

B

C

α=0.1, β=1.0, k/k'=10

α=1.0, β=0.1, k/k'=10

α=1.0, β=1.0, k/k'=1

α=0.01, β=1.0, k/k'=10

α=1.0, β=0.01, k/k'=10

α=1.0, β=1.0, k/k'=100

Concentration: 3.0e+00, 2.5, 2, 1.5, 1, 0.5, 0.0e+00

Figure S1. Parameter analysis in the single pipe geometry. The distribution of concentration affected by different settings of (A) penalty parameter α for the cost to control high concentration gradient; (B) penalty parameter β for the cost of control force; and (C) the ratio between attachment rate k and detachment rate k'. Unit for color bars: $mol/\mu m^3$.

A

B

C

α=0.01

α=0.1

α=1.0

β=0.01

β=0.1

β=1.0

Velocity: 1.0, 0.8, 0.6, 0.4, 0.2, 0

D

E

F

α=0.01

α=0.1

α=1.0

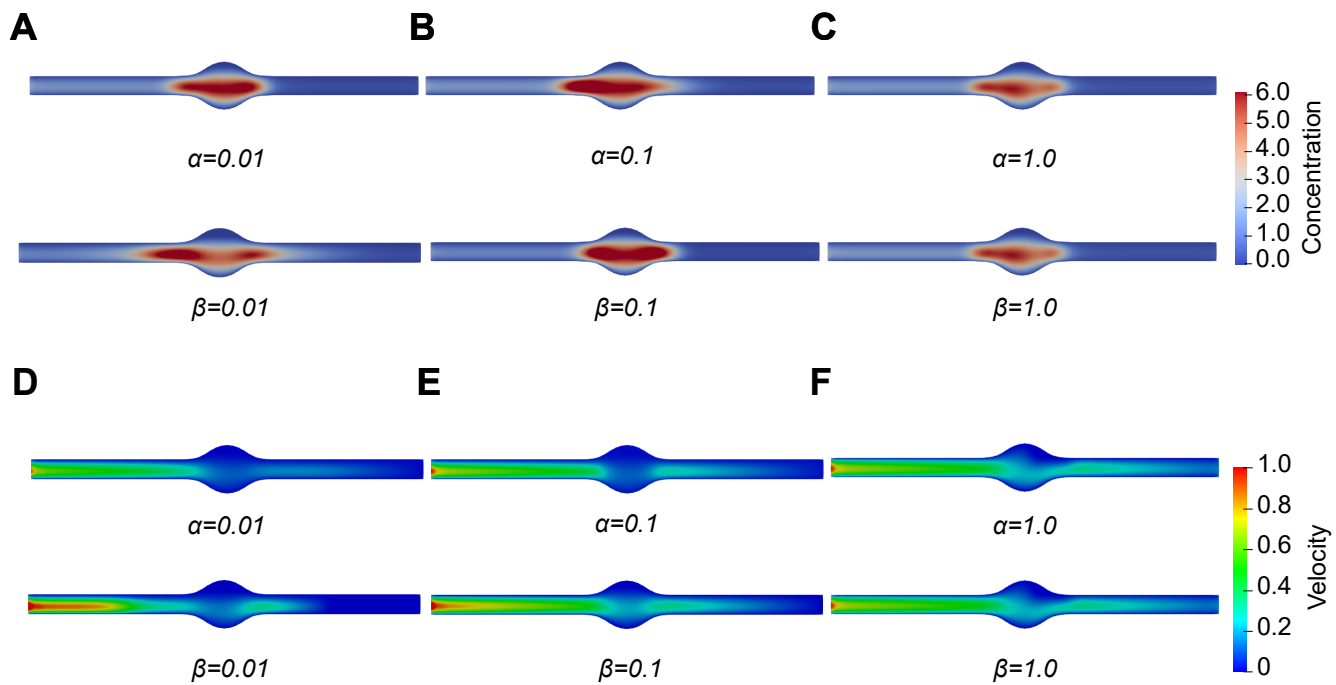β=0.01

β=0.1

β=1.0

force: 0.05, 0.04, 0.03, 0.02, 0.01, 0

Figure S2. Simulation results in the single pipe geometry with different settings of penalty parameter α and β. (A-C) Computed velocity field. (D-F) The distribution of control force. Unit for color bars: Velocity: $\mu m/s$; Control force: $\mu m/s^2$.
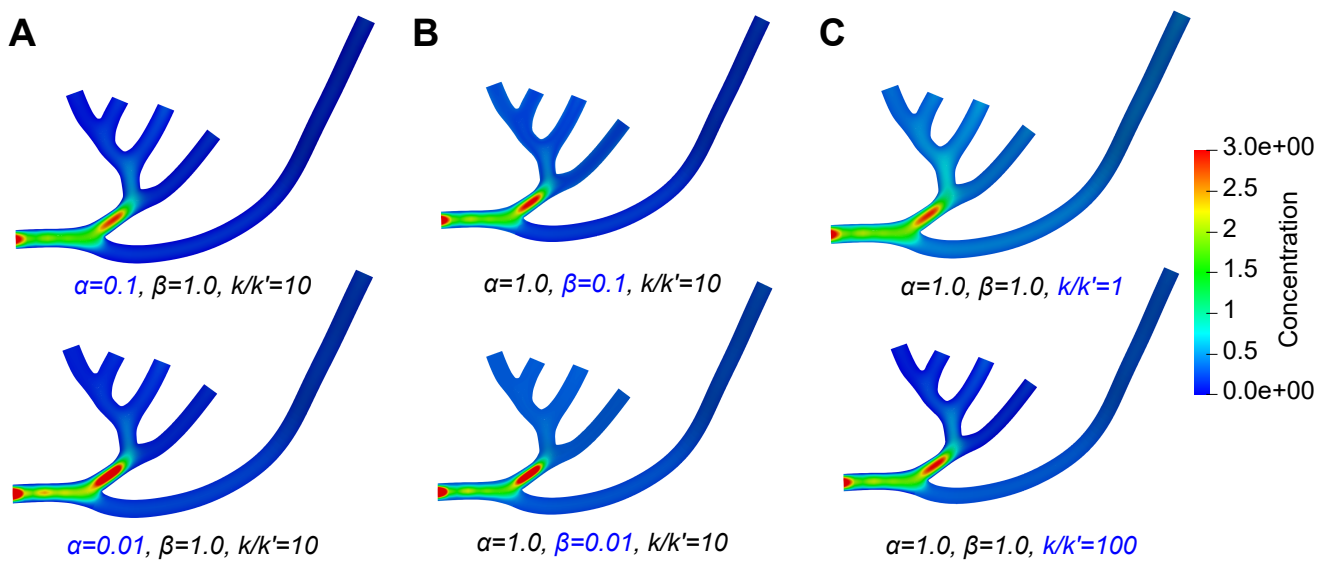
Figure S3. Parameter analysis in the neuron tree extracted from NMO_54504. The distribution of concentration affected by different settings of (A) penalty parameter α for the cost to control high concentration gradient; (B) penalty parameter β for the cost of control force; and (C) the ratio between attachment rate k and detachment rate k'. Unit for color bars: $mol/\mu m^3$.
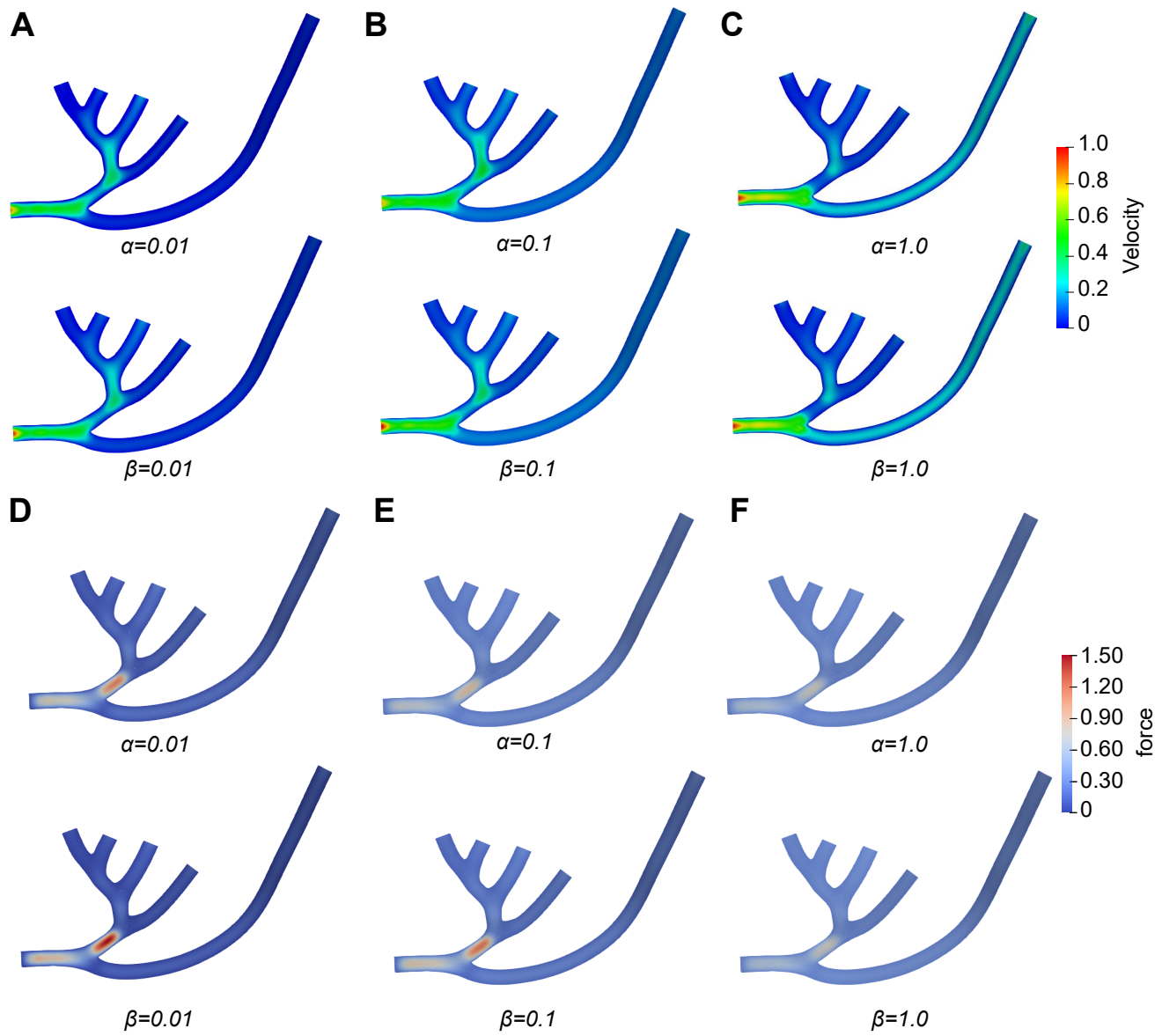
Figure S4. Simulation results in the neuron tree extracted from NMO_54504 with different settings of penalty parameter α and β. (A-C) Computed velocity field. (D-F) The distribution of control force. Unit for color bars: Velocity: $\mu m/s$; Control force: $\mu m/s^2$.

Figure S5. Simulation results in the pipe with swelling geometry with different settings of penalty parameter α and β. (A-C) Material distribution. (D-F) Computed velocity field. Unit for color bars: Concentration: $mol/\mu m^3$; Velocity: $\mu m/s$.
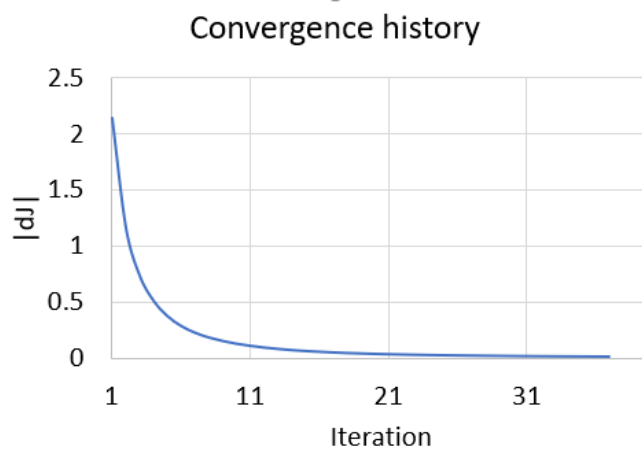
Figure S6. The convergence history of the simulation in single pipe geometry.