Benchmark problem #6

Solved with MOOSE framework

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Cahn-Hilliard equation

- Strong form

$$\frac{\partial c}{\partial t} = \nabla \cdot M(c)\nabla\mu$$

$$\mu = \frac{\delta F}{\delta c} = \frac{\partial f_{chem}}{\partial c} + \frac{\partial f_{elec}}{\partial c} - \kappa\nabla^2 c$$

- Weak form; 'forward split' method

$$\nabla\mu \cdot \vec{n} = 0$$

$$R_c = \int_\Omega \left(\frac{\partial c}{\partial t} - \nabla \cdot M(c)\nabla\mu\right)\psi_c d\Omega = \int_\Omega \frac{\partial c}{\partial t}\psi_c d\Omega + \int_\Omega M(c)\nabla\mu \cdot \nabla\psi_c d\Omega = 0$$

with $\int_A \psi_\mu M(c)\nabla\mu \cdot d\vec{A} = 0$

$$R_\mu = \int_\Omega \left(-\mu + \frac{\partial f_{chem}}{\partial c} + \frac{\partial f_{elec}}{\partial c} - \kappa\nabla^2 c\right)\psi_\mu d\Omega = \int_\Omega \left(-\mu + \frac{\partial f_{chem}}{\partial c} + \frac{\partial f_{elec}}{\partial c}\right)\psi_\mu d\Omega + \int_\Omega \kappa\nabla c \cdot \nabla\psi_\mu d\Omega = 0$$

with $\int_A \psi_\mu \kappa\nabla c \cdot d\vec{A} = 0$

Poisson equation for Φ_{tot}; natural BC

- Strong form

$$\nabla \cdot \epsilon \nabla(\Phi_{ext} + \Phi_{int}) = -k(c - c_0)$$

- Weak form

$$R_{\Phi_{int}} = \int_\Omega [\nabla \cdot \epsilon \nabla(\Phi_{ext} + \Phi_{int}) + k(c - c_0)]\psi_{\Phi_{int}} d\Omega$$

$$= \int_A \psi_c \epsilon \nabla(\Phi_{ext} + \Phi_{int}) \cdot d\vec{A} - \int_\Omega \epsilon \nabla(\Phi_{ext} + \Phi_{int}) \cdot \nabla \psi_{\Phi_{int}} d\Omega + \int_\Omega k(c - c_0)\psi_{\Phi_{int}} d\Omega$$

$$= -\int_\Omega \epsilon \nabla(\Phi_{ext} + \Phi_{int}) \cdot \nabla \psi_{\Phi_{int}} d\Omega + \int_\Omega k(c - c_0)\psi_{\Phi_{int}} d\Omega = 0$$

with $\int_A \psi_c \epsilon \nabla(\Phi_{ext} + \Phi_{int}) \cdot d\vec{A} = 0 \quad \longleftarrow \quad \nabla(\Phi_{ext} + \Phi_{int}) \cdot \vec{n} = 0 \qquad \Phi_{int}(50, 50) = 0$

Poisson equation for Φ_{int}; Neuman BC

- Strong form

$$\nabla \cdot \epsilon \nabla \Phi_{int} = -k(c - c_0)$$

- Weak form

$$R_{\Phi_{int}} = \int_\Omega [\nabla \cdot \epsilon \nabla \Phi_{int} + k(c - c_0)] \psi_{\Phi_{int}} d\Omega$$

$$= \int_A \psi_c \epsilon \nabla \Phi_{int} \cdot d\vec{A} - \int_\Omega \epsilon \nabla \Phi_{int} \cdot \nabla \psi_{\Phi_{int}} d\Omega + \int_\Omega k(c - c_0) \psi_{\Phi_{int}} d\Omega = 0$$

$$= -\int_A \psi_c \epsilon \nabla \Phi_{ext} \cdot d\vec{A} - \int_\Omega \epsilon \nabla \Phi_{int} \cdot \nabla \psi_{\Phi_{int}} d\Omega + \int_\Omega k(c - c_0) \psi_{\Phi_{int}} d\Omega = 0$$

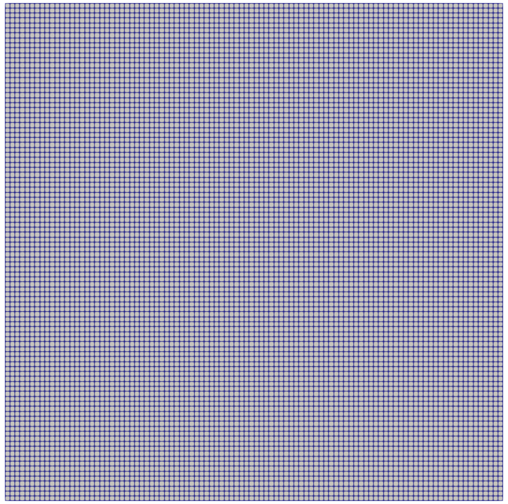
$$\nabla(\Phi_{ext} + \Phi_{int}) \cdot \vec{n} = 0$$

$$\Phi_{int}(1, 1) = 0$$

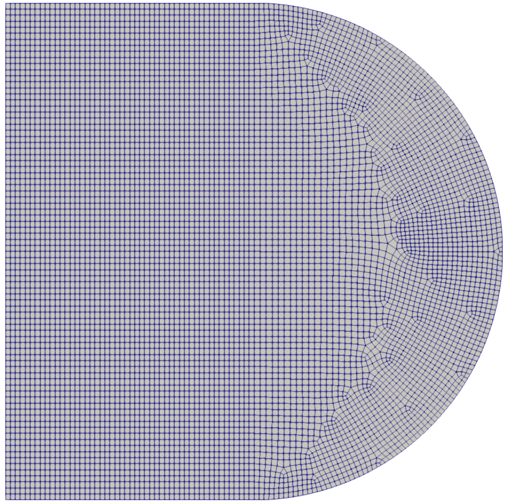
Discretization & numerical parameters

- Element type: quadrilateral with 4 nodes
- Element size: 1
- Time step: adaptive time steps with initially 10^{-5} to maximum 5.
- Time step growth factor: 1.8
- Time step cutback factor: 0.5
- Residual tolerance: 10^{-9}

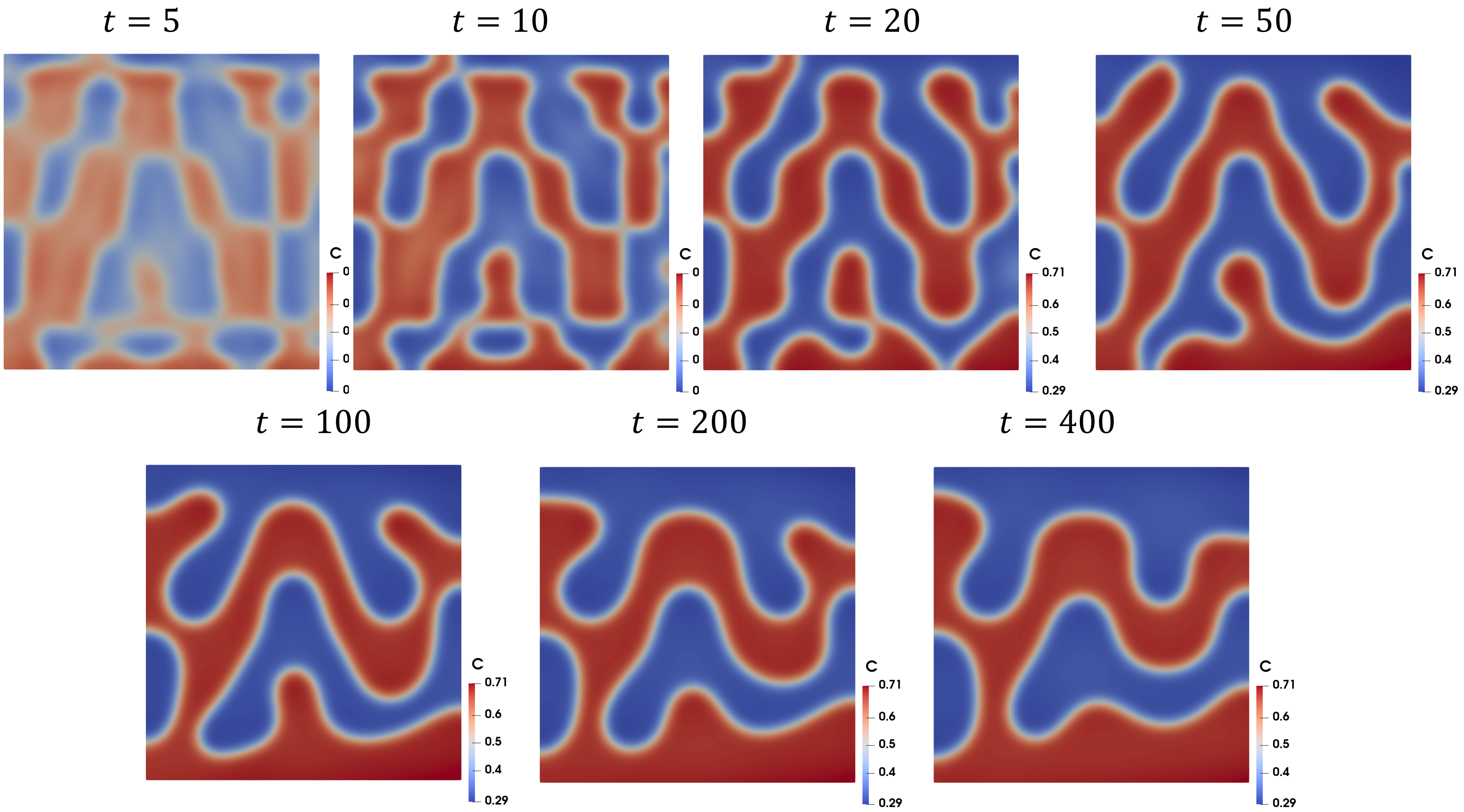
(a)



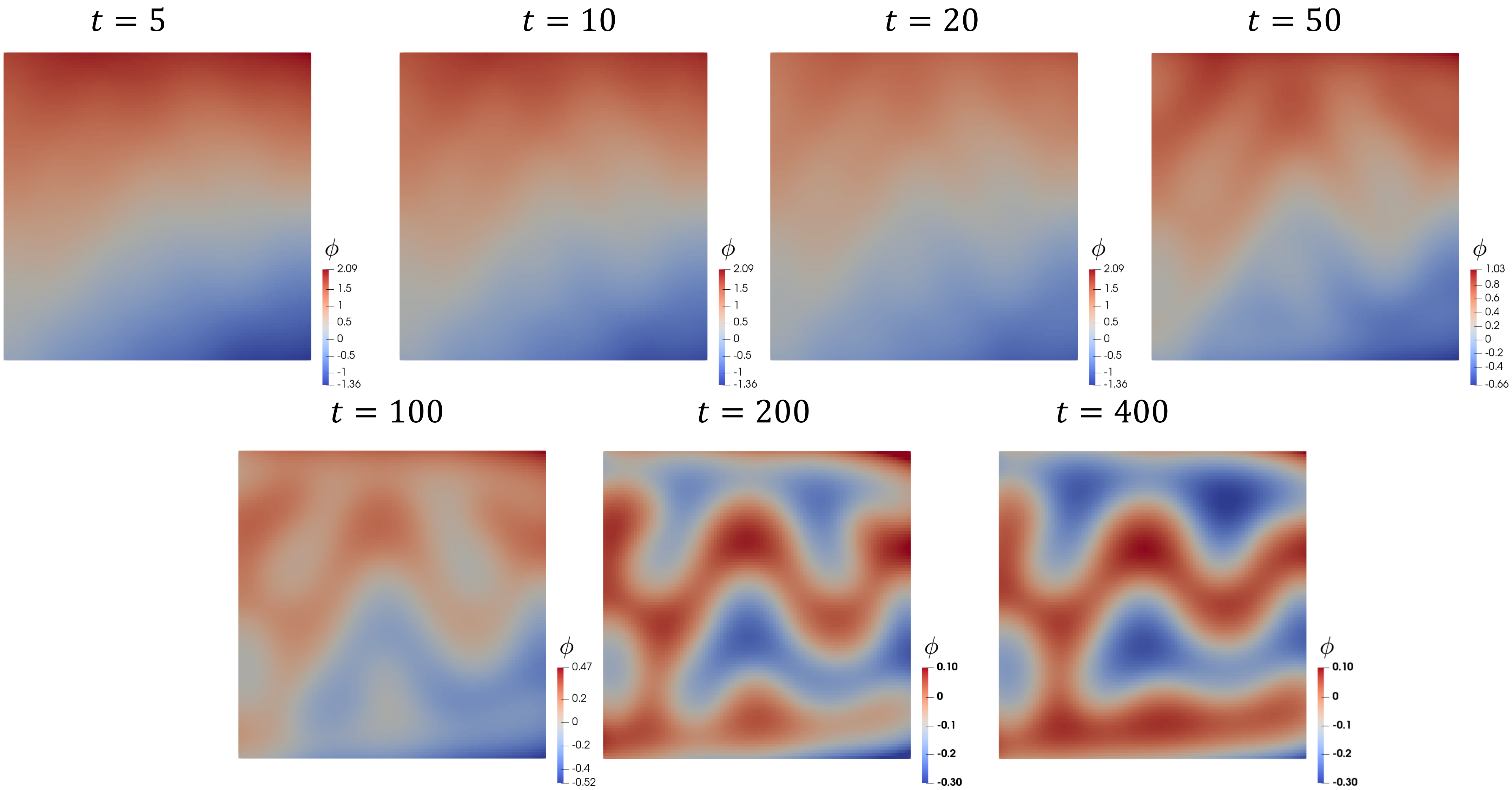
(b)



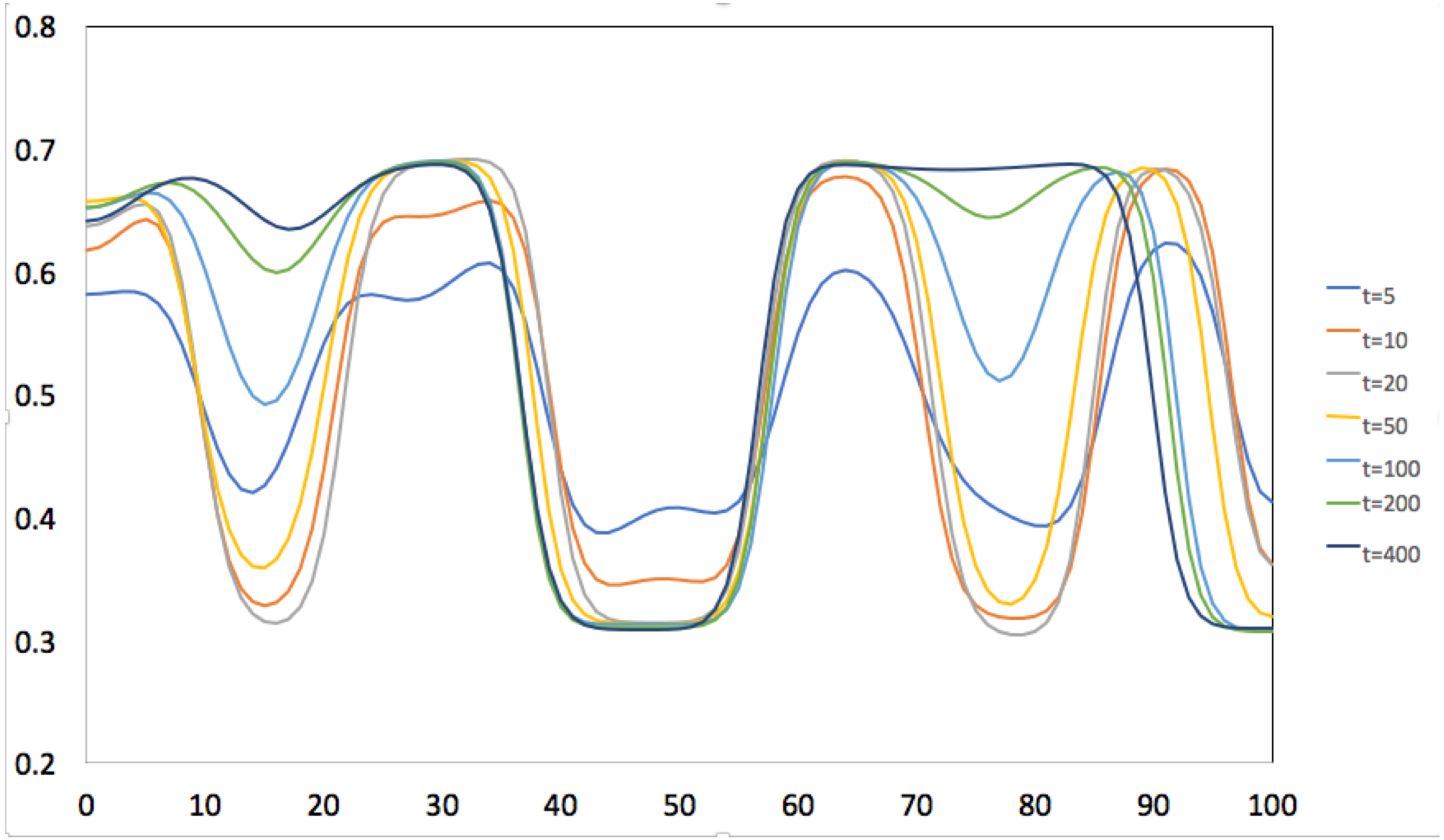
Results for (a) with function Neumann B.C: concentration field



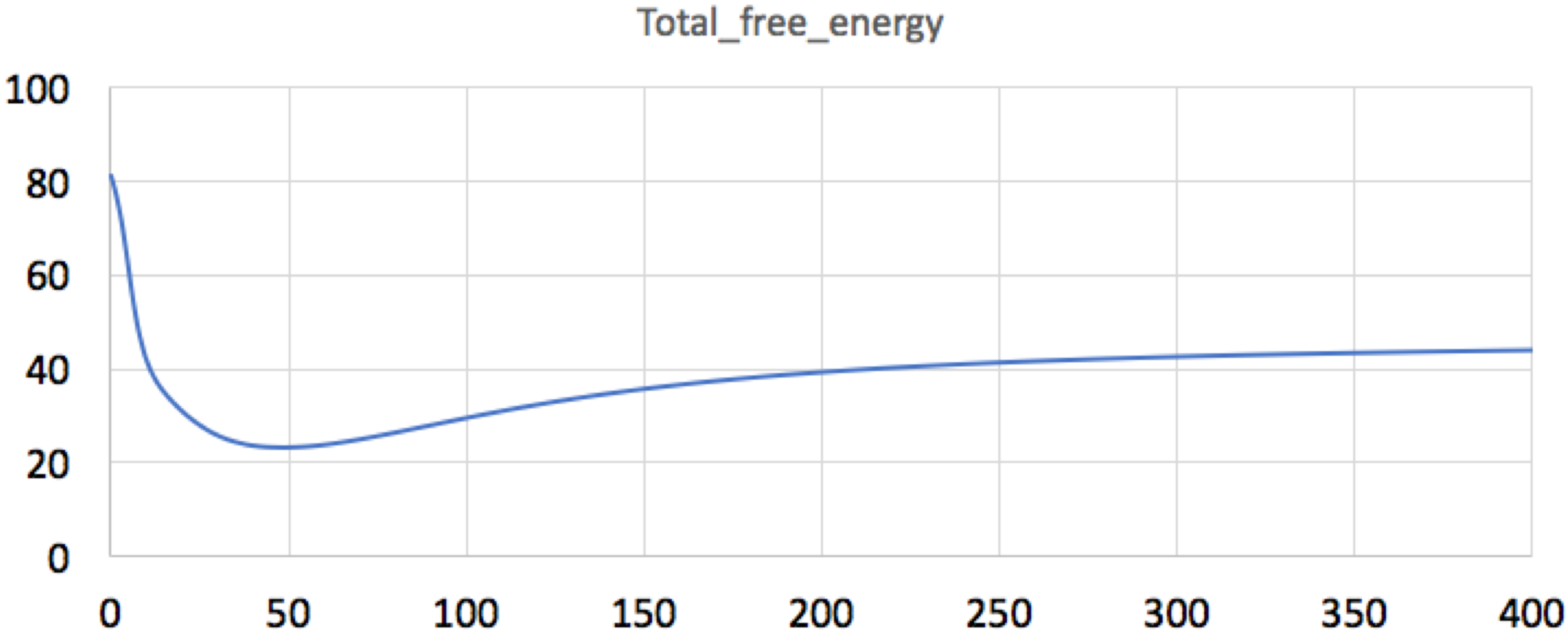
Results for (a)-Function Neumann B.C: Electric potential field



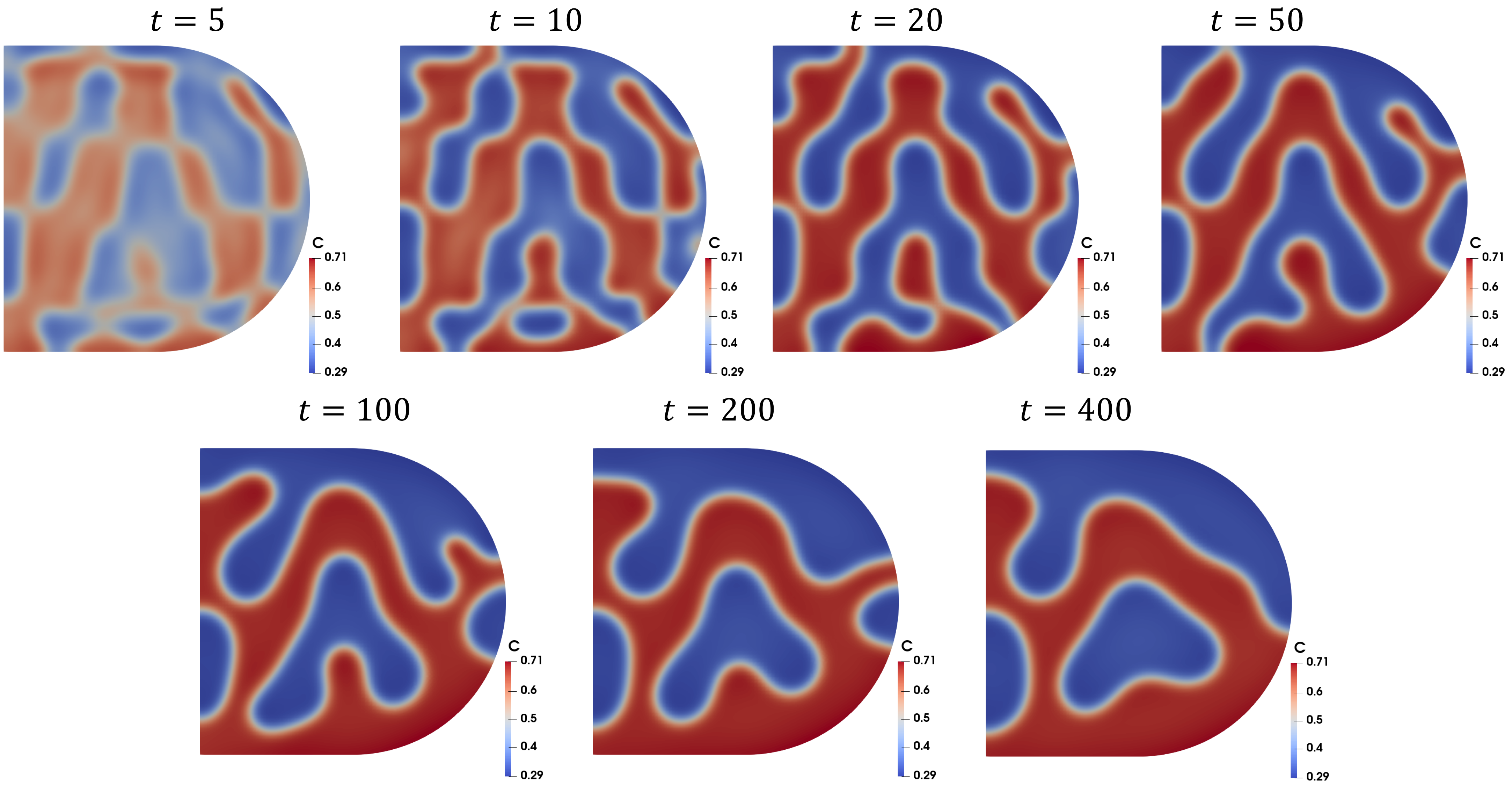
Results for (a)-Function Neumann B.C: cross-sectional concentration



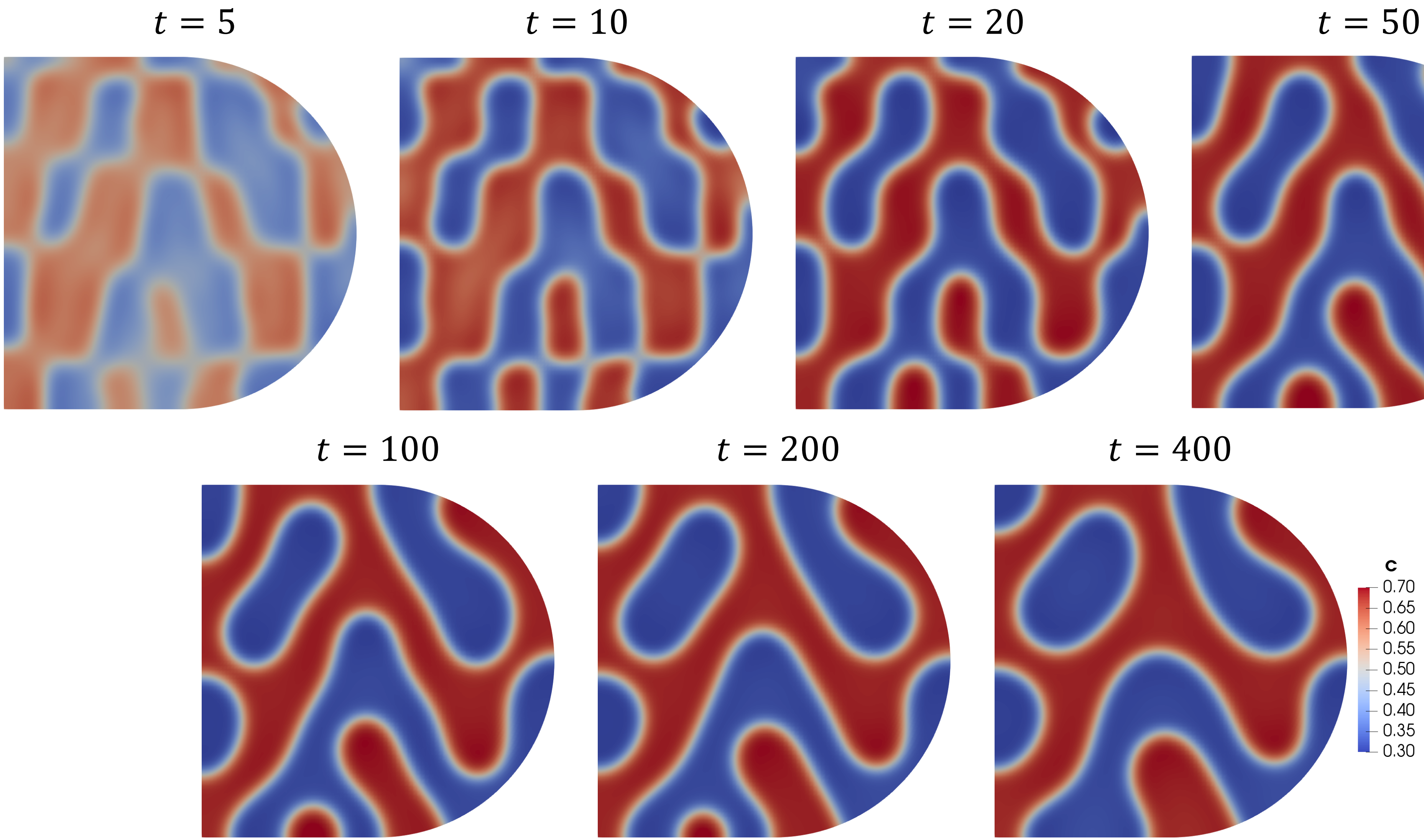
Results for (a)- Function Neumann B.C. total free energy



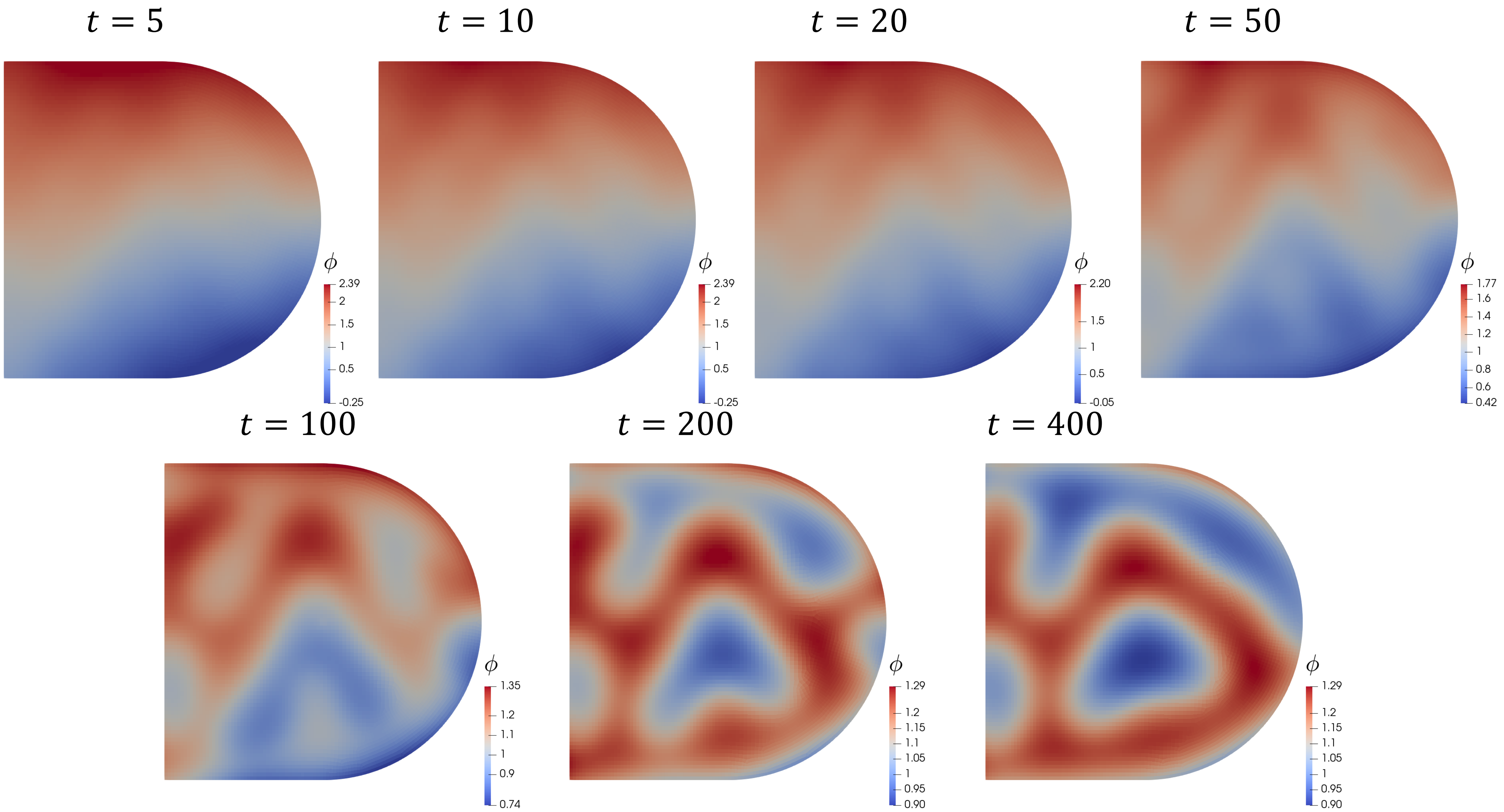
Results for (b)—Neumann B.C.: concentration field



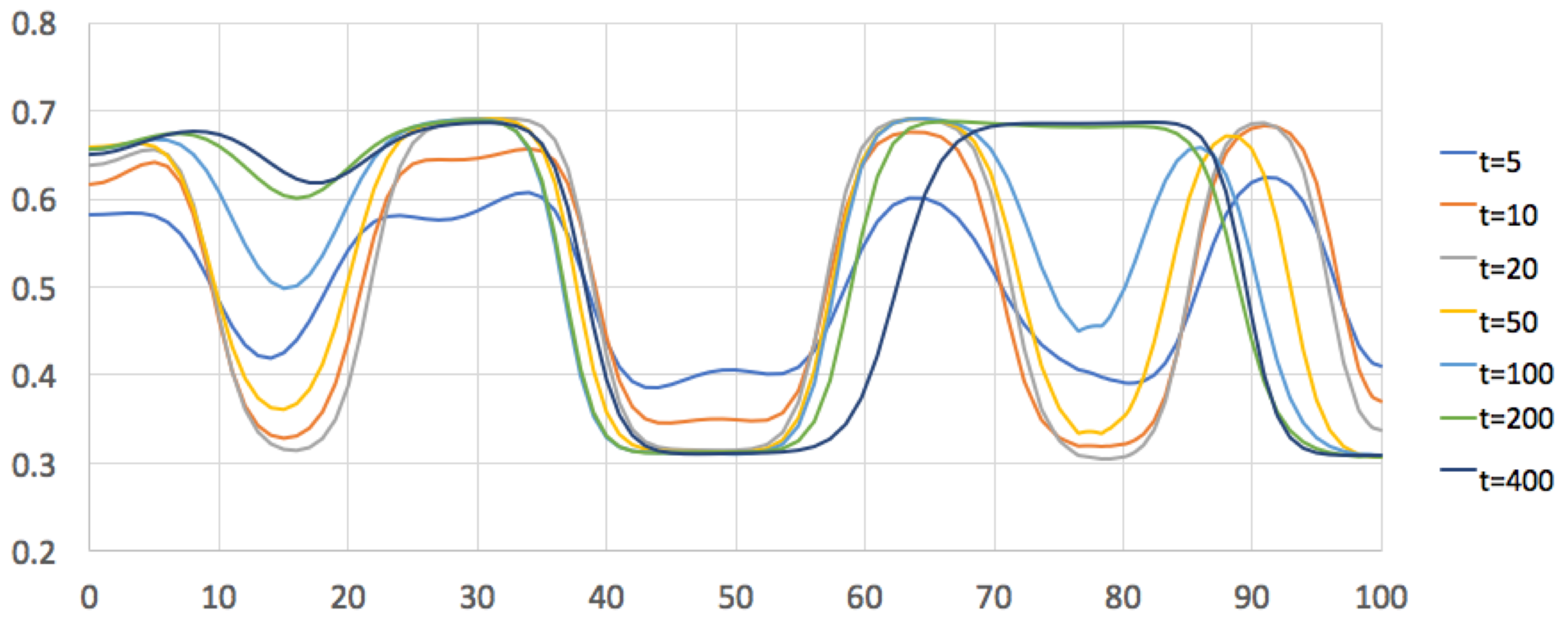
Results for (b): concentration field



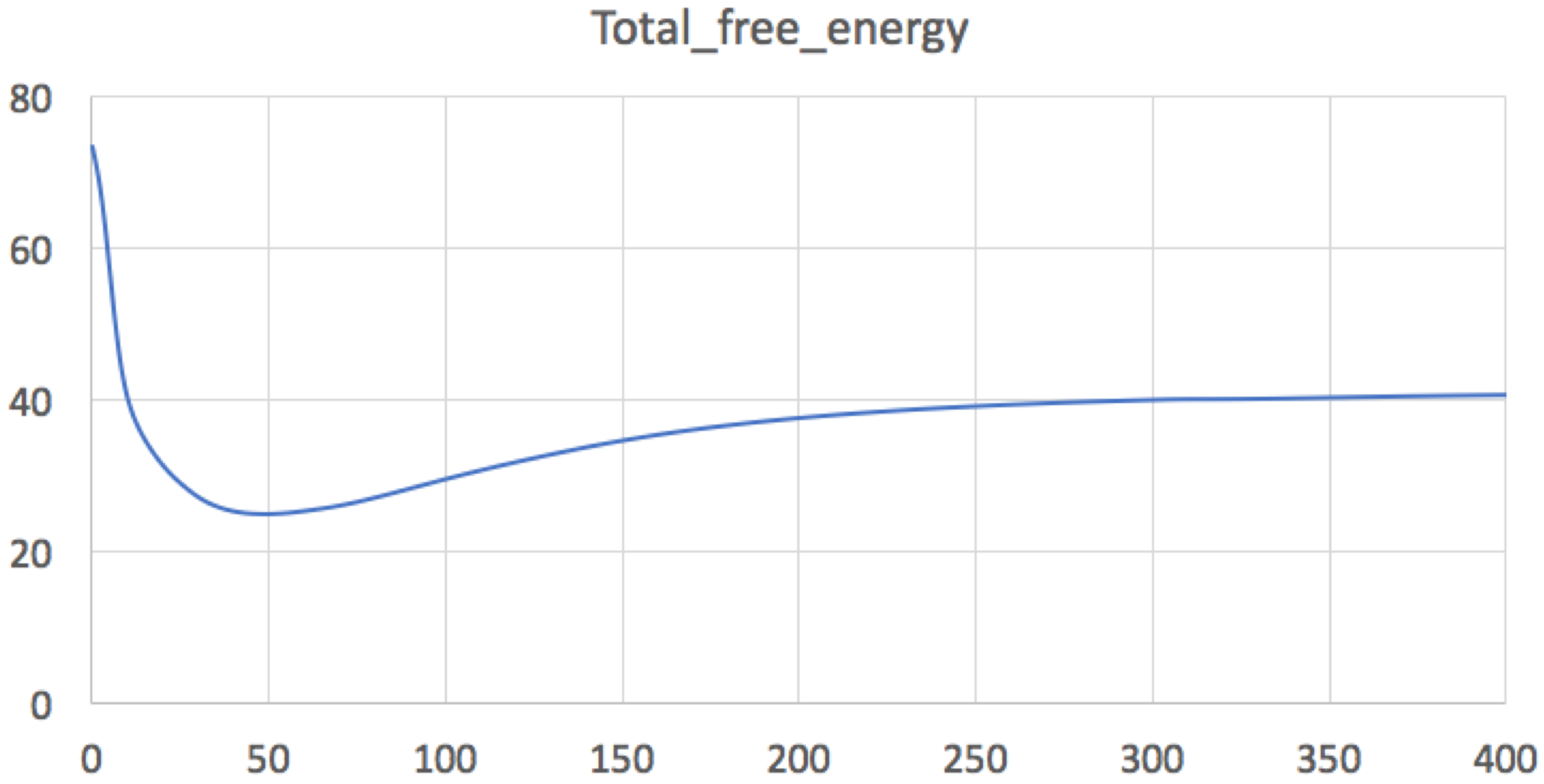
Results for (b)—Neumann B.C.
Electric potential field



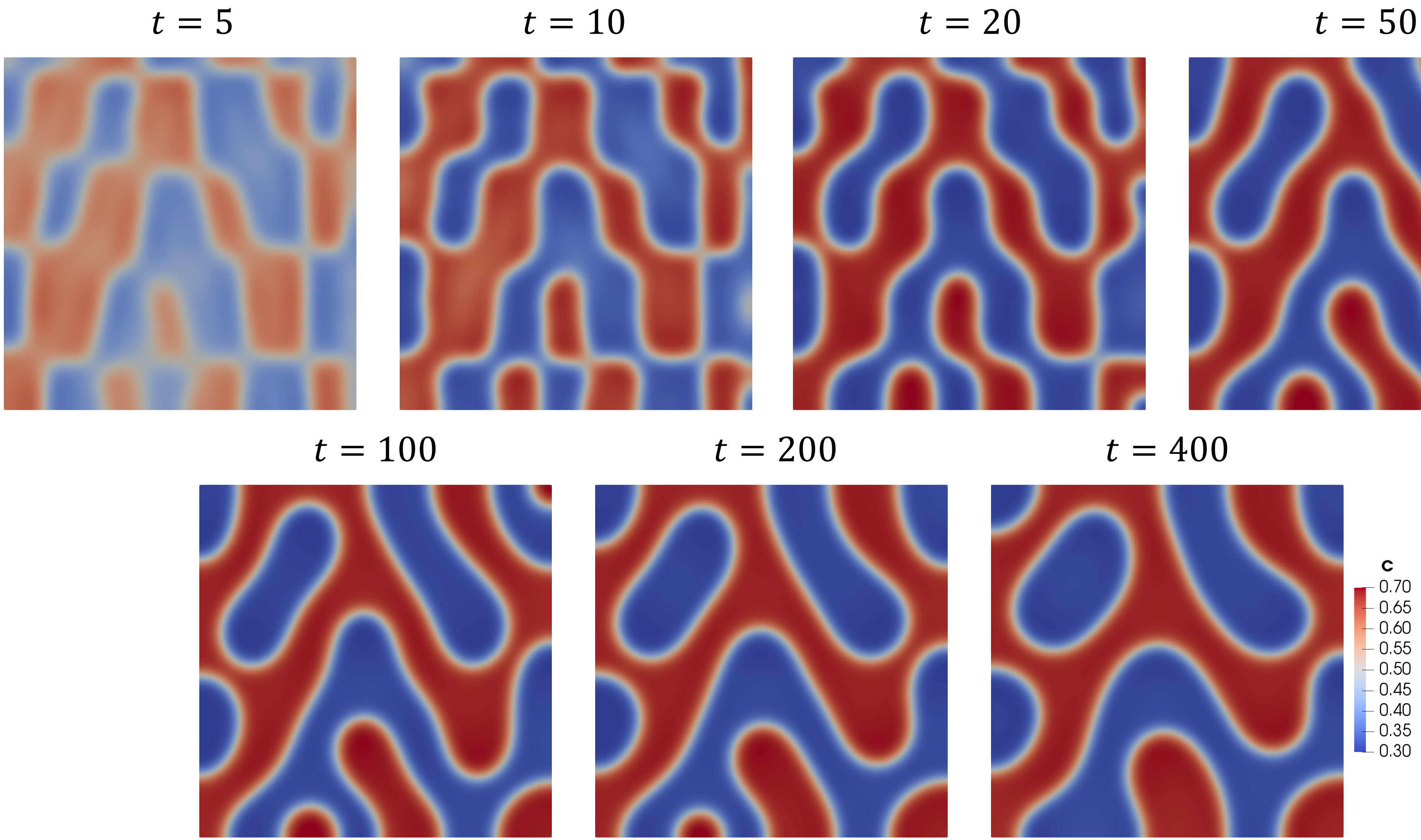
Results for (b)—Neuman B.C.: cross-sectional concentration



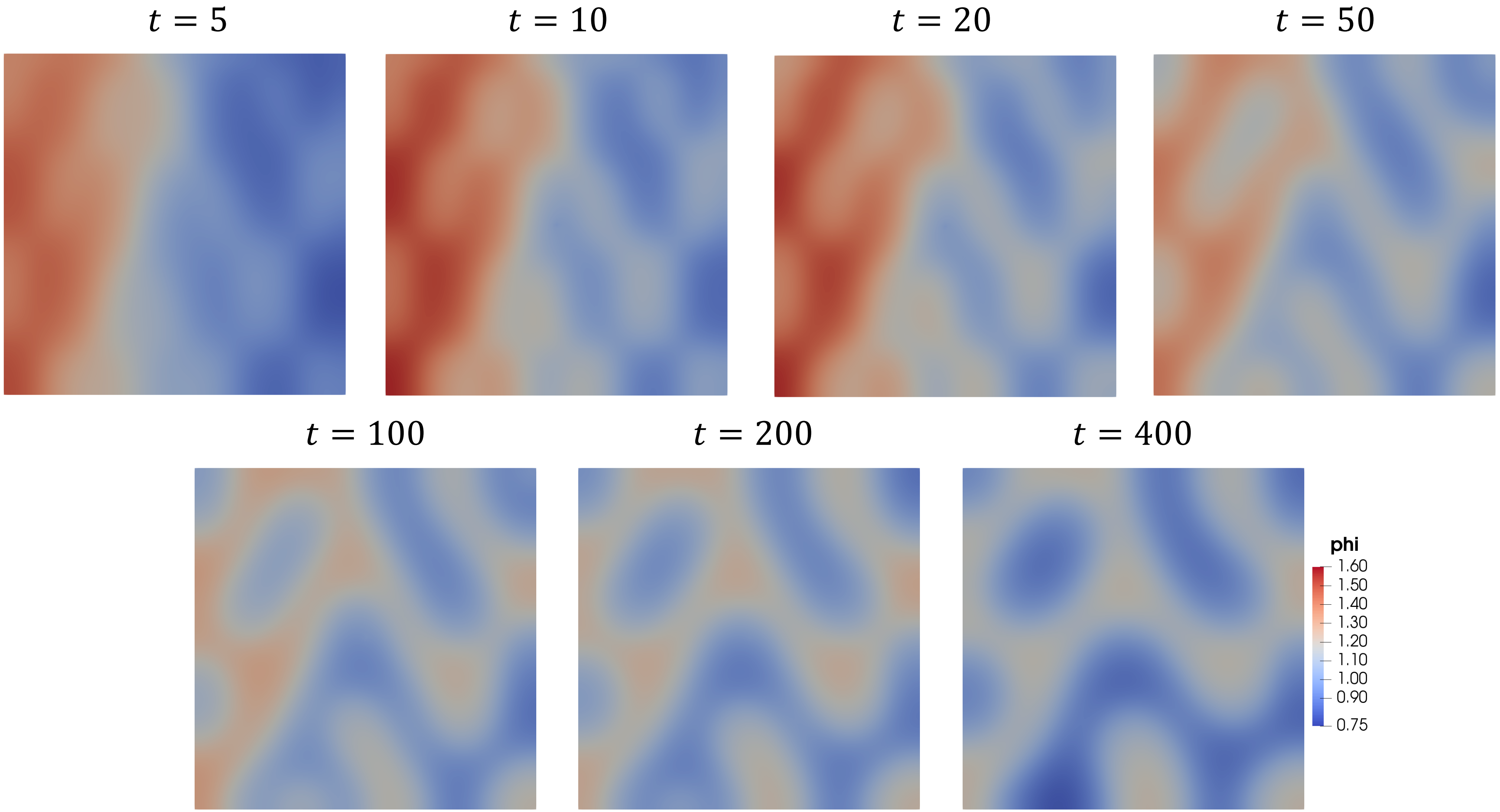
Results for (b)—Neumann B.C. total free energy



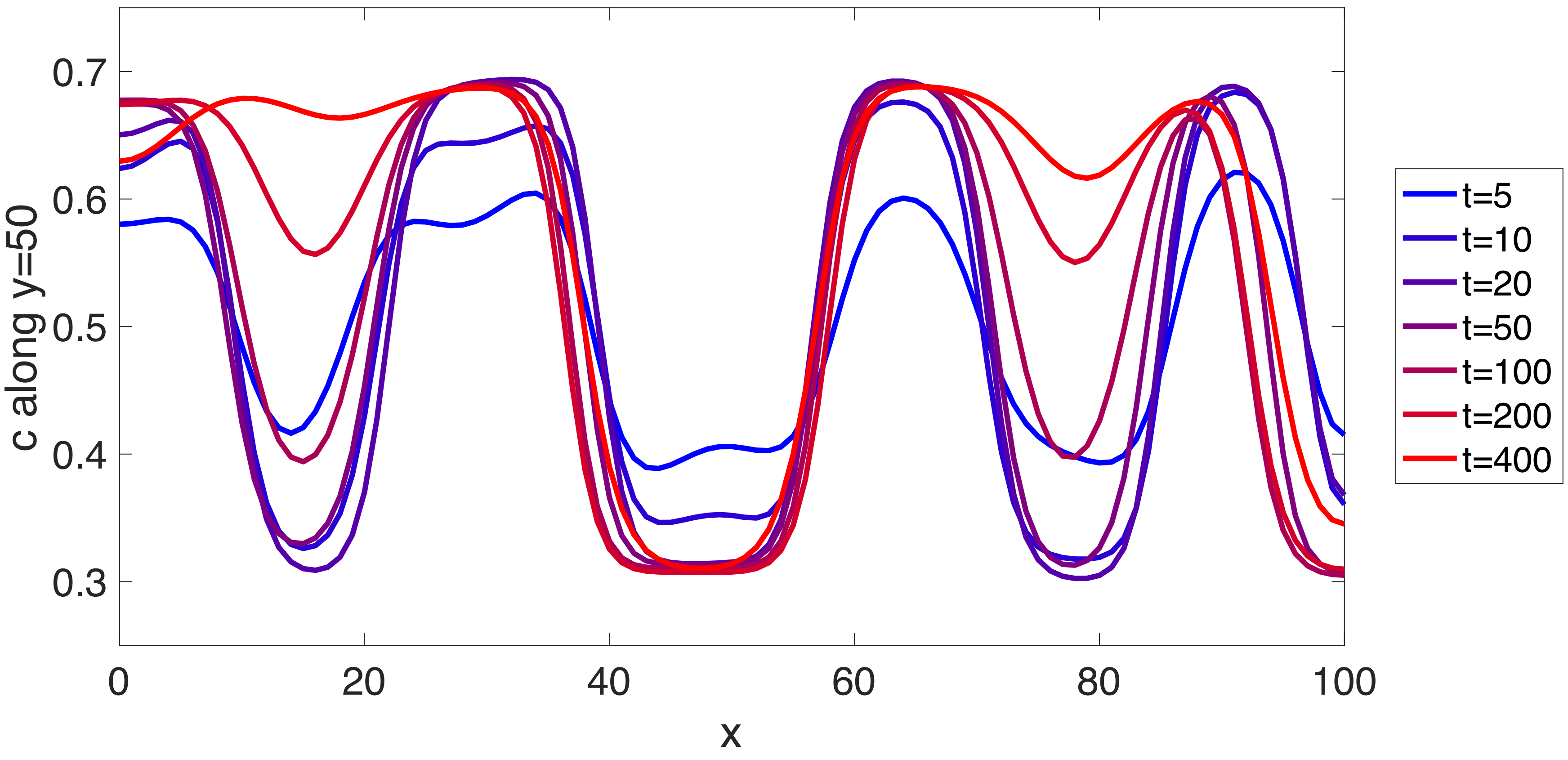
Results for (a): concentration field



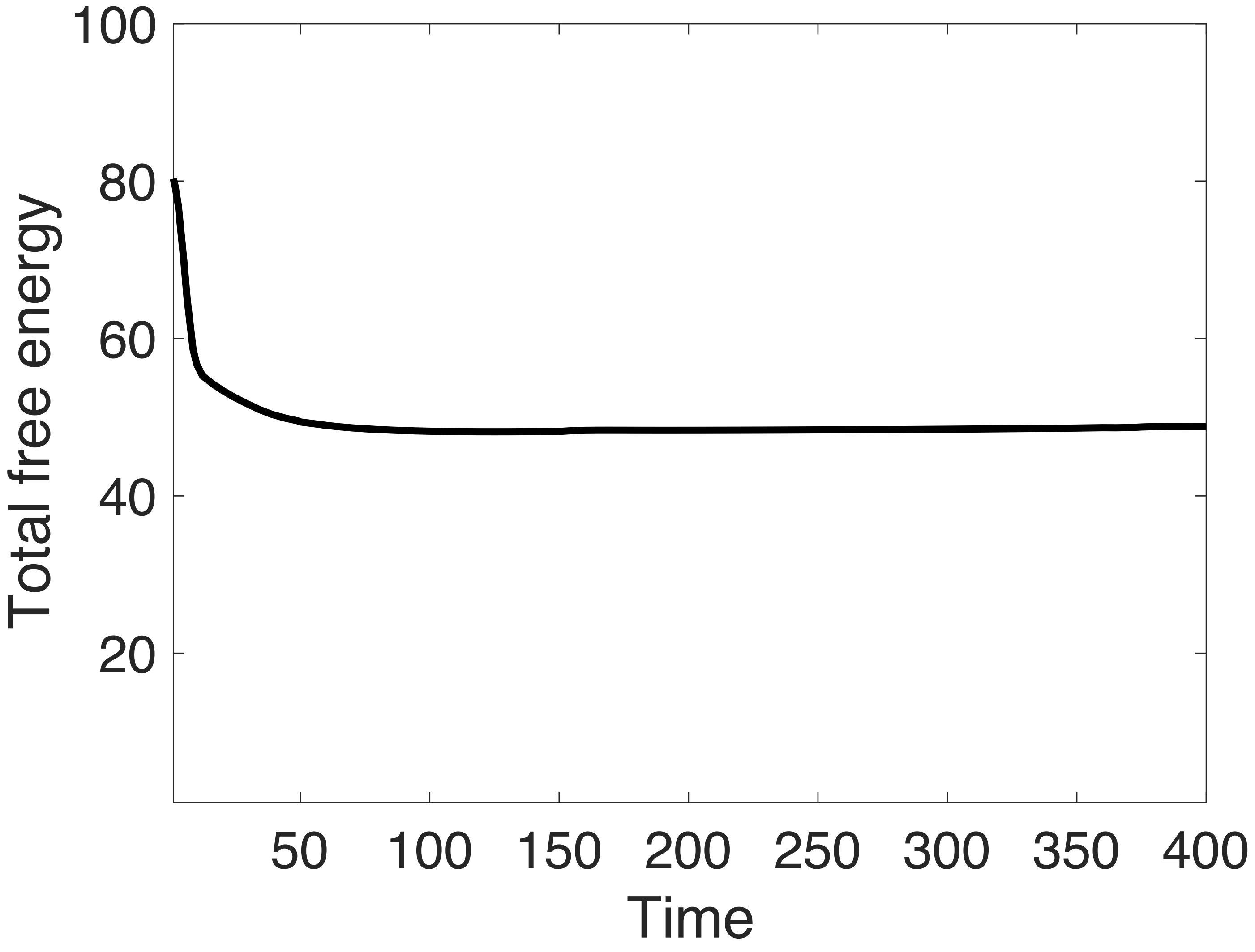
Results for (a): Electric potential field



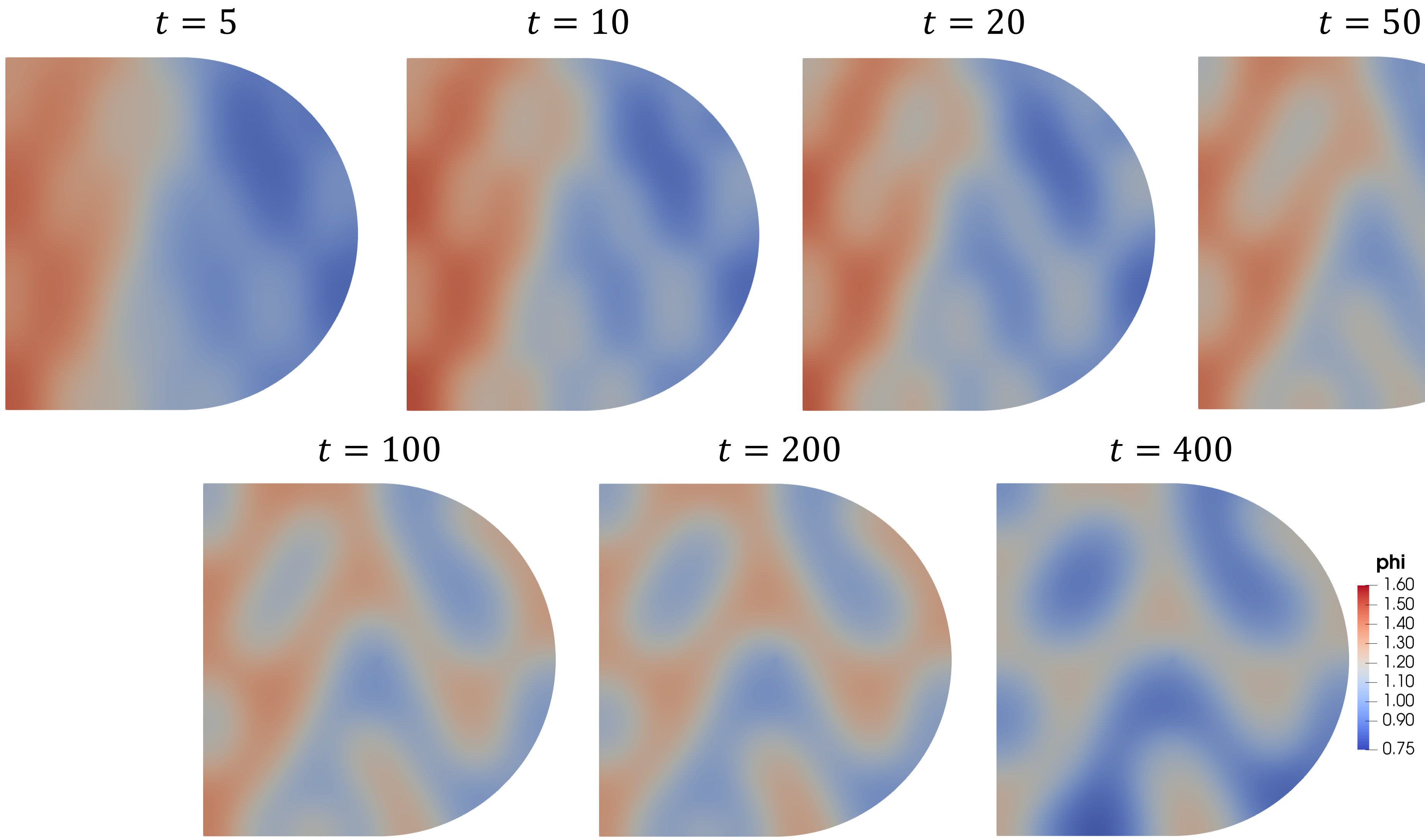
Results for (a): cross-sectional concentration



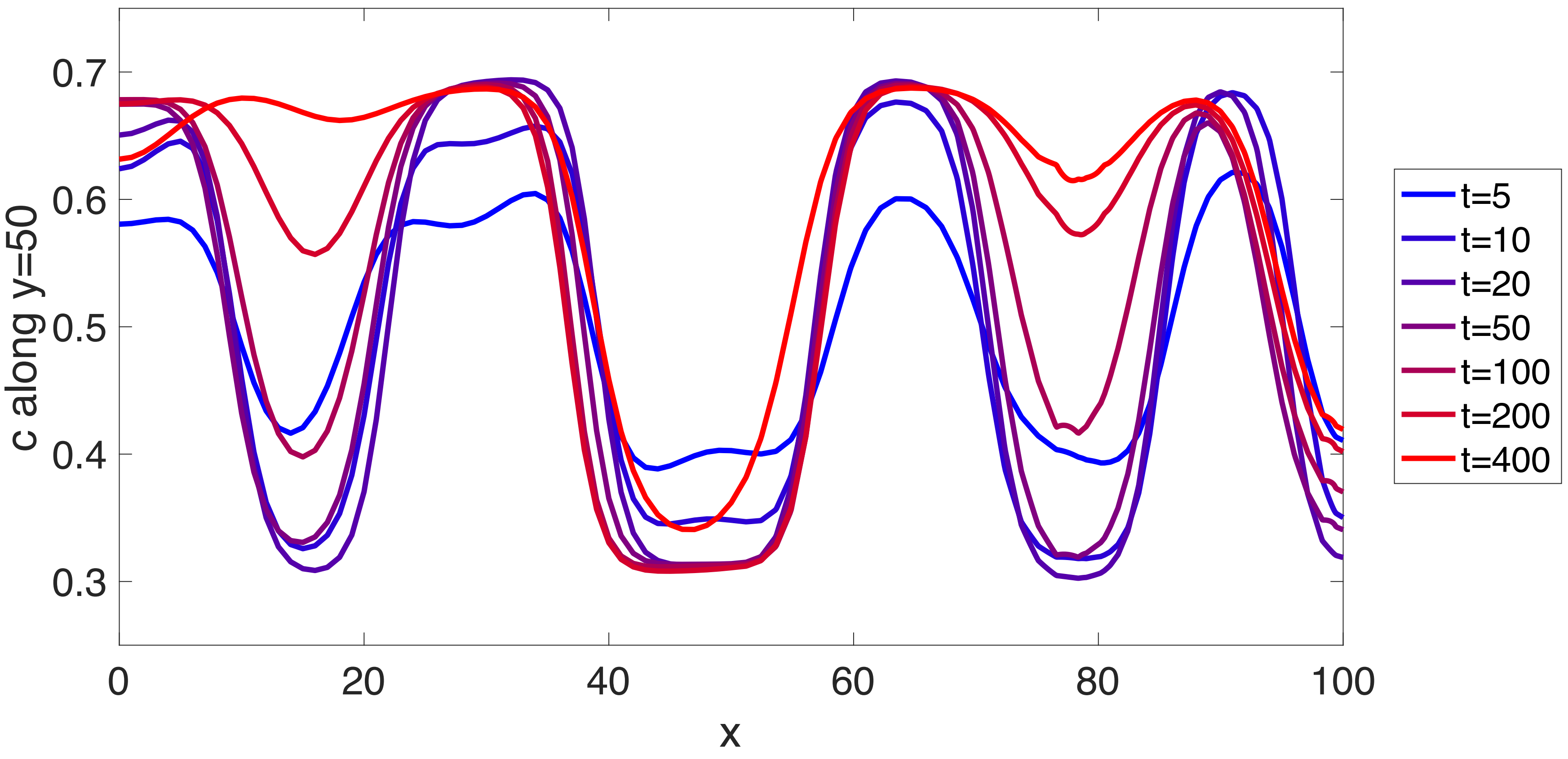
Results for (a): total free energy



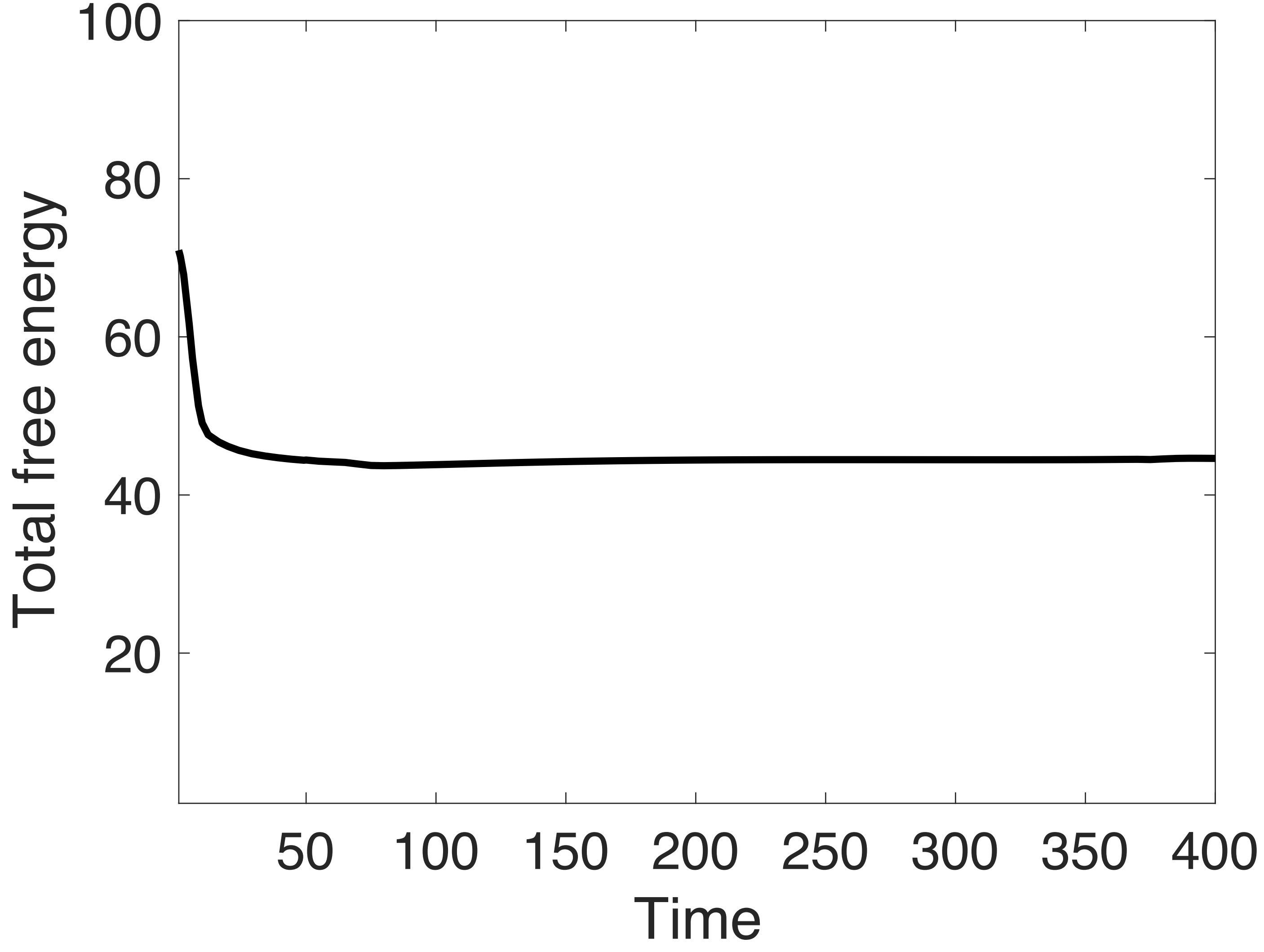
Results for (b): Electric potential field



Results for (b): cross-sectional concentration



Results for (b): total free energy



Discussion about total free energy change

$$F = \int_V \frac{\kappa}{2}|\nabla c|^2 + f_{chem}(c) + f_{elec}(c,\Phi)dV$$

$$\frac{\partial F}{\partial t} = \int_V \mu\frac{\partial c}{\partial t} + \frac{\delta F}{\delta \Phi}\frac{\partial \Phi}{\partial t}dV = \int_V \mu\nabla\cdot M\nabla\mu + \frac{\rho_{tot}}{2}\frac{\partial \Phi}{\partial t}dV$$

$$= \int_V -M(\nabla\mu)^2 + \frac{1}{2}\epsilon\nabla^2\Phi\frac{\partial \Phi}{\partial t}dV = \int_V -M(\nabla\mu)^2 - \frac{1}{2}\epsilon\nabla\Phi\cdot\frac{\partial\nabla\Phi}{\partial t}dV$$

$$= \int_V -M(\nabla\mu)^2 - \frac{1}{4}\epsilon\frac{\partial}{\partial t}(\nabla\Phi)^2 dV$$

Is this always positive?

Discussion about electrostatic free energy density

$$\epsilon \nabla^2 \Phi = -k(c - c_0)$$

With BC: $\nabla \Phi \cdot \vec{n} = 0$

$$\epsilon \nabla^2 (\Phi + C) = -k(c - c_0)$$

$$\nabla (\Phi + C) \cdot \vec{n} = 0$$

C: arbitrary constant

$$f_{elec}(c, \Phi) = \frac{1}{2} k(c - c_0)(\Phi + C)$$

Probably we need to take control of C.