

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

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

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



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

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

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

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

Poisson equation for Φ_{int} ; Neuman BC

- Strong form

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

- Weak form

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

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

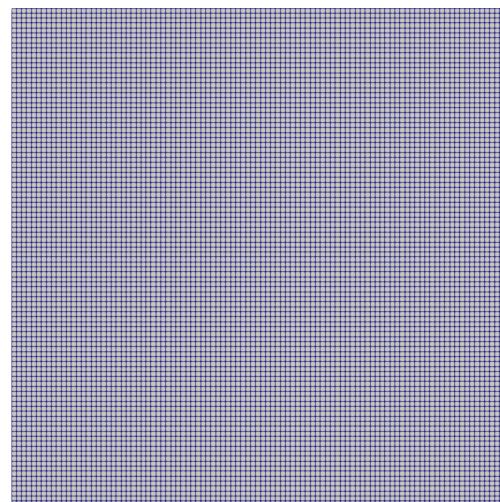
$$= - \int_A \psi_c \epsilon \nabla \Phi_{ext} \cdot d\vec{A} - \int_{\Omega} \epsilon \nabla \Phi_{int} \cdot \nabla \psi_{\Phi_{int}} d\Omega + \int_{\Omega} k(c - c_0) \psi_{\Phi_{int}} d\Omega = 0$$

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

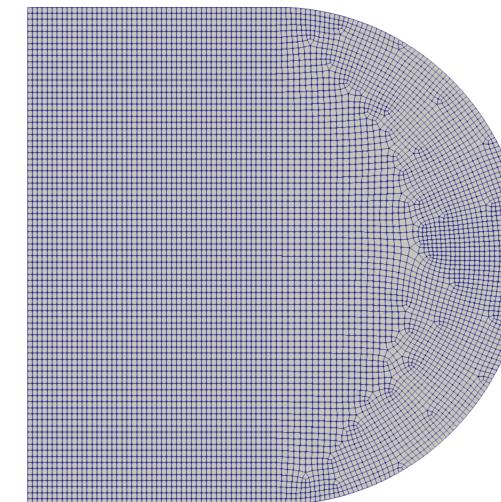
Discretization & numerical parameters

- 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}

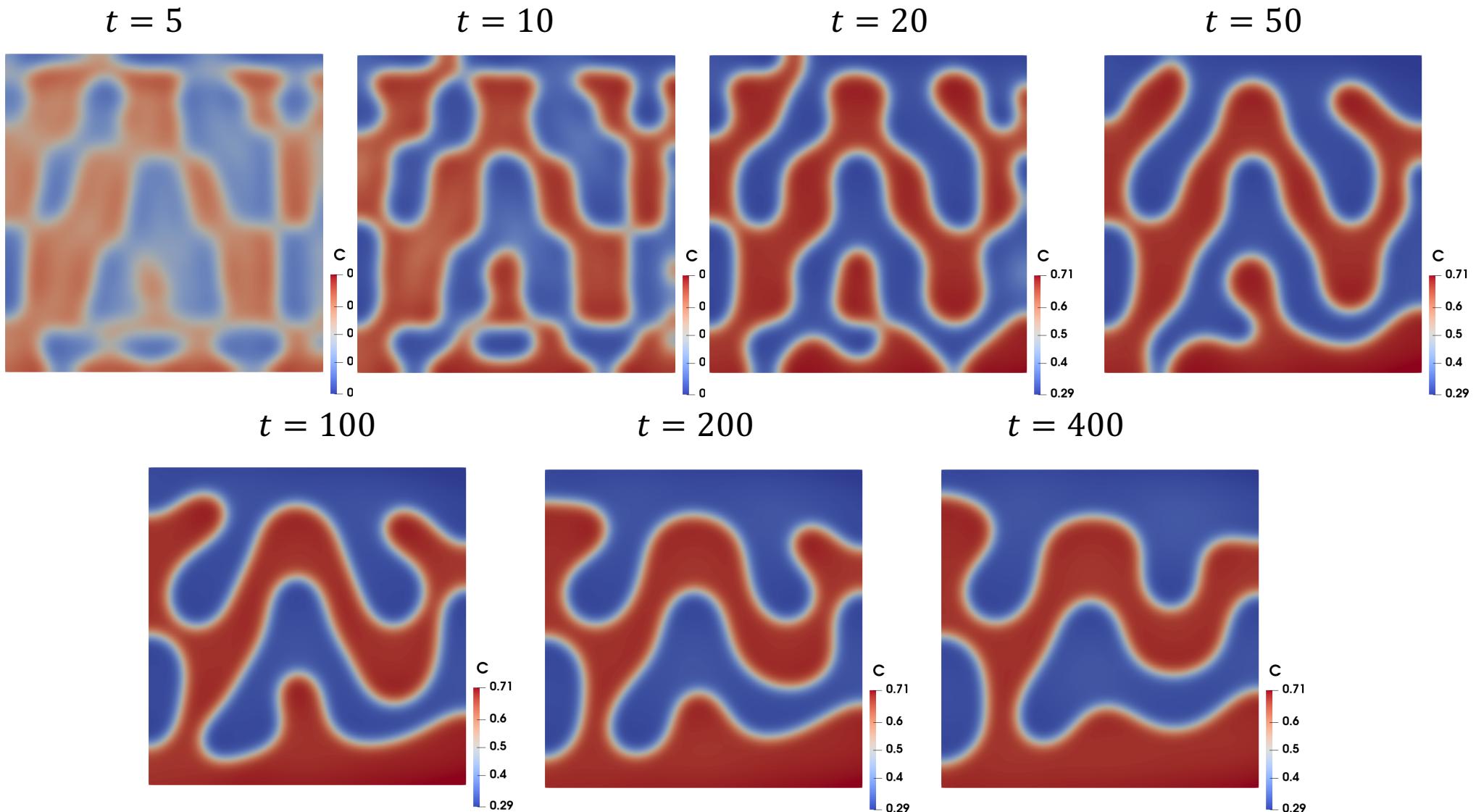
(a)



(b)

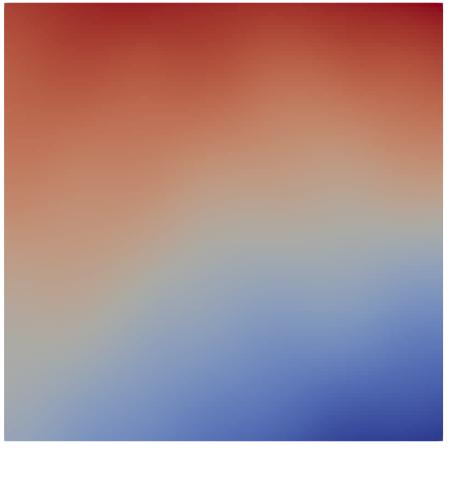


Results for (a) with function Neumann B.C:
concentration field

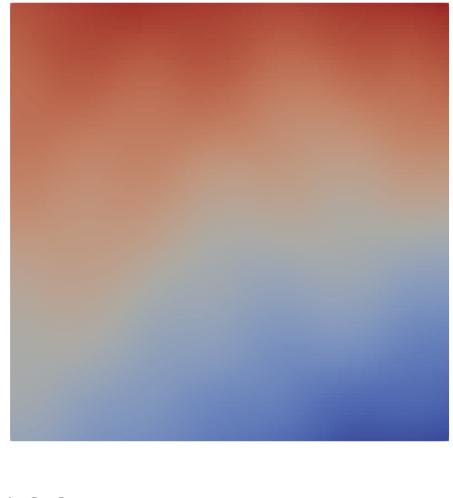


Results for (a)-Function Neumann B.C: Electric potential field

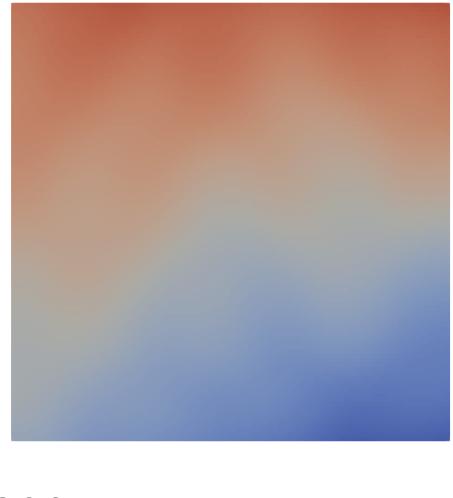
$t = 5$



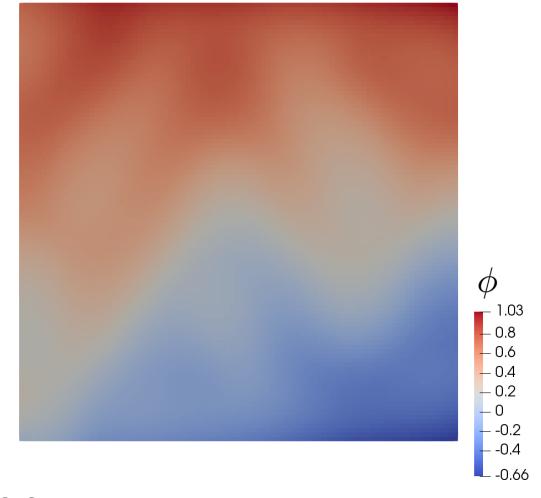
$t = 10$



$t = 20$



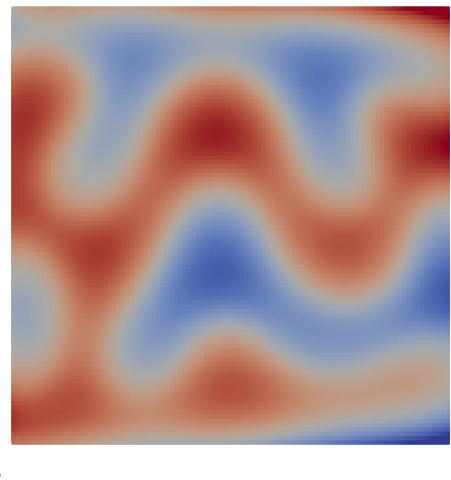
$t = 50$



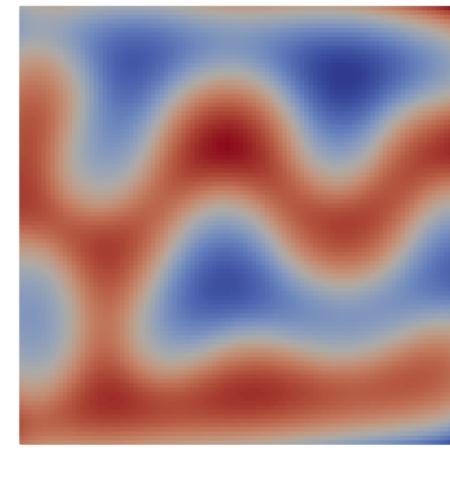
$t = 100$



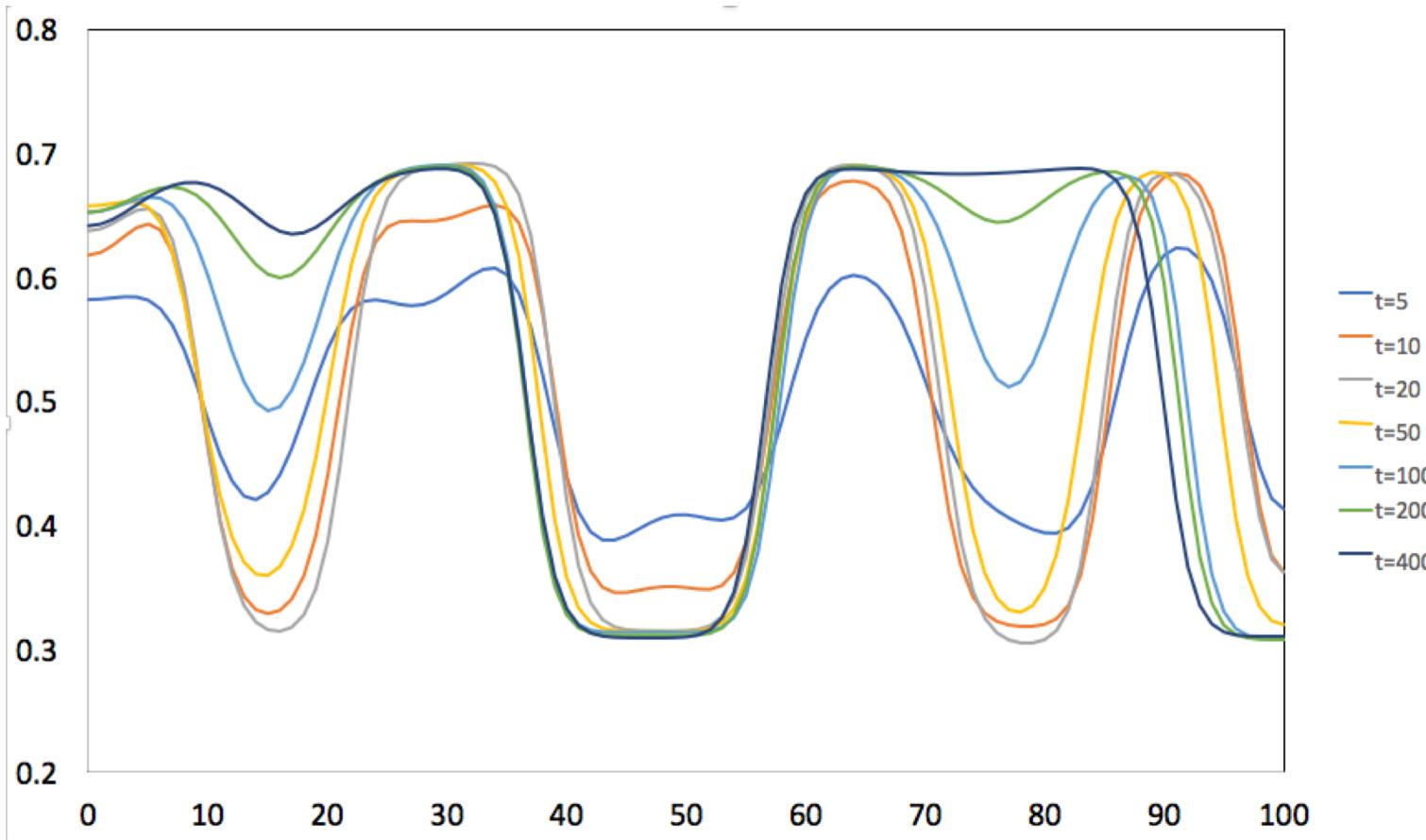
$t = 200$



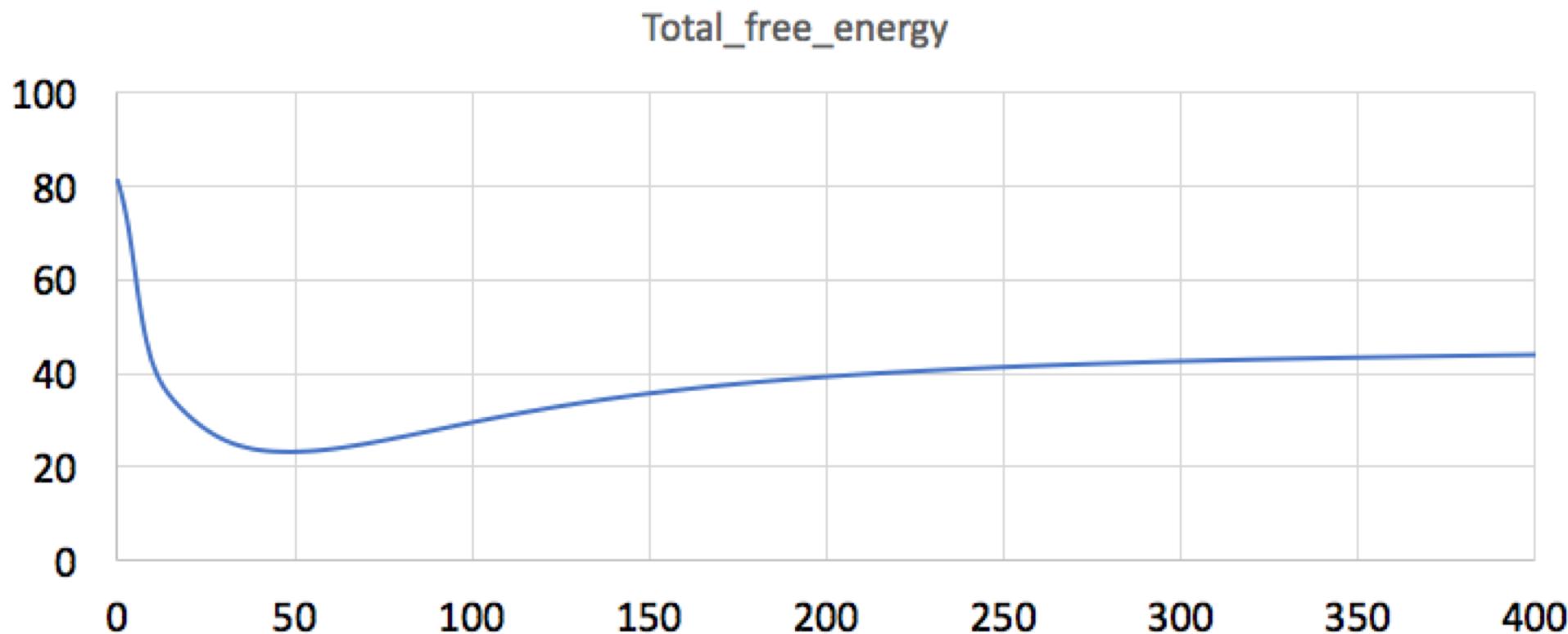
$t = 400$



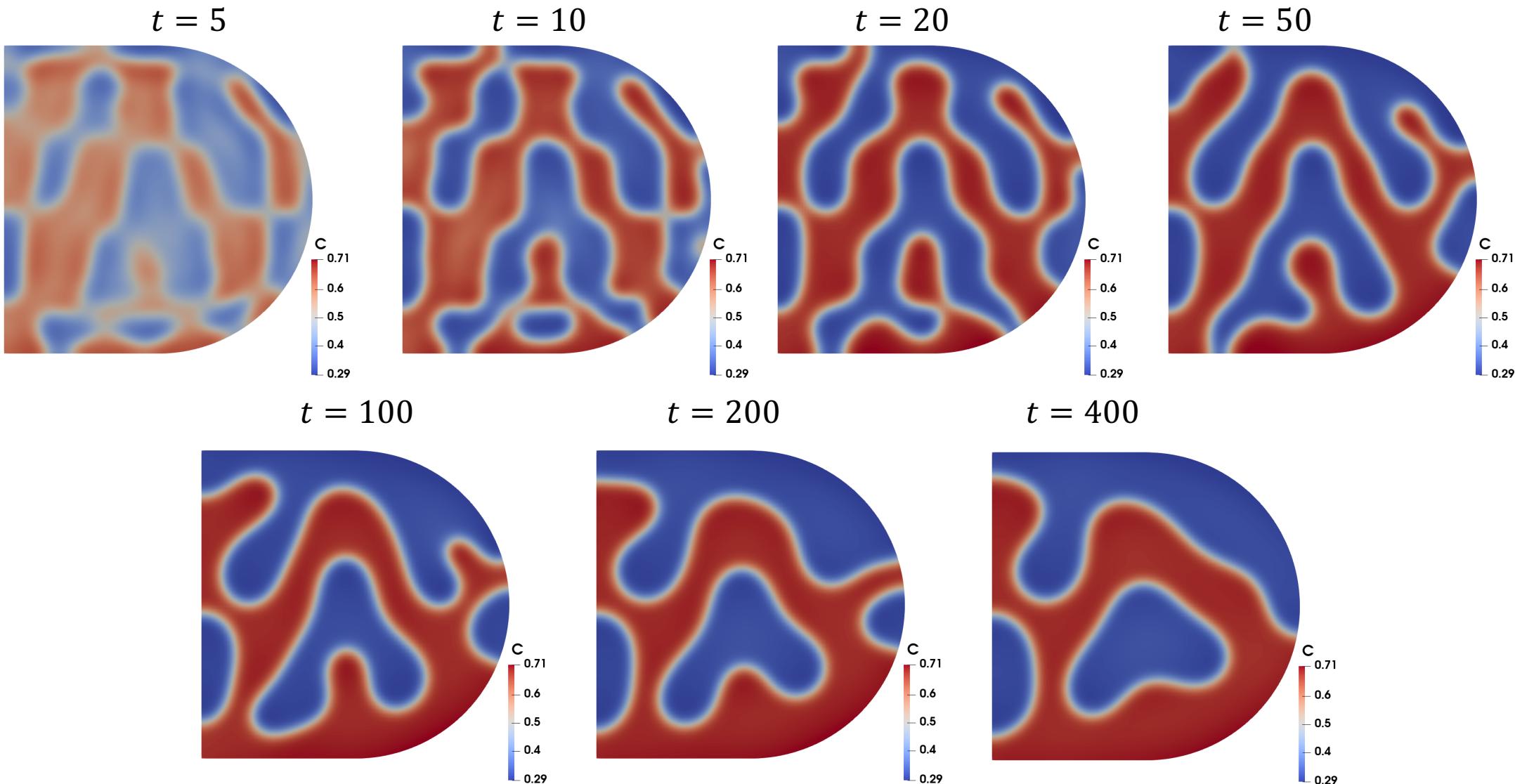
Results for (a)-Function Neumann B.C: cross-sectional concentration



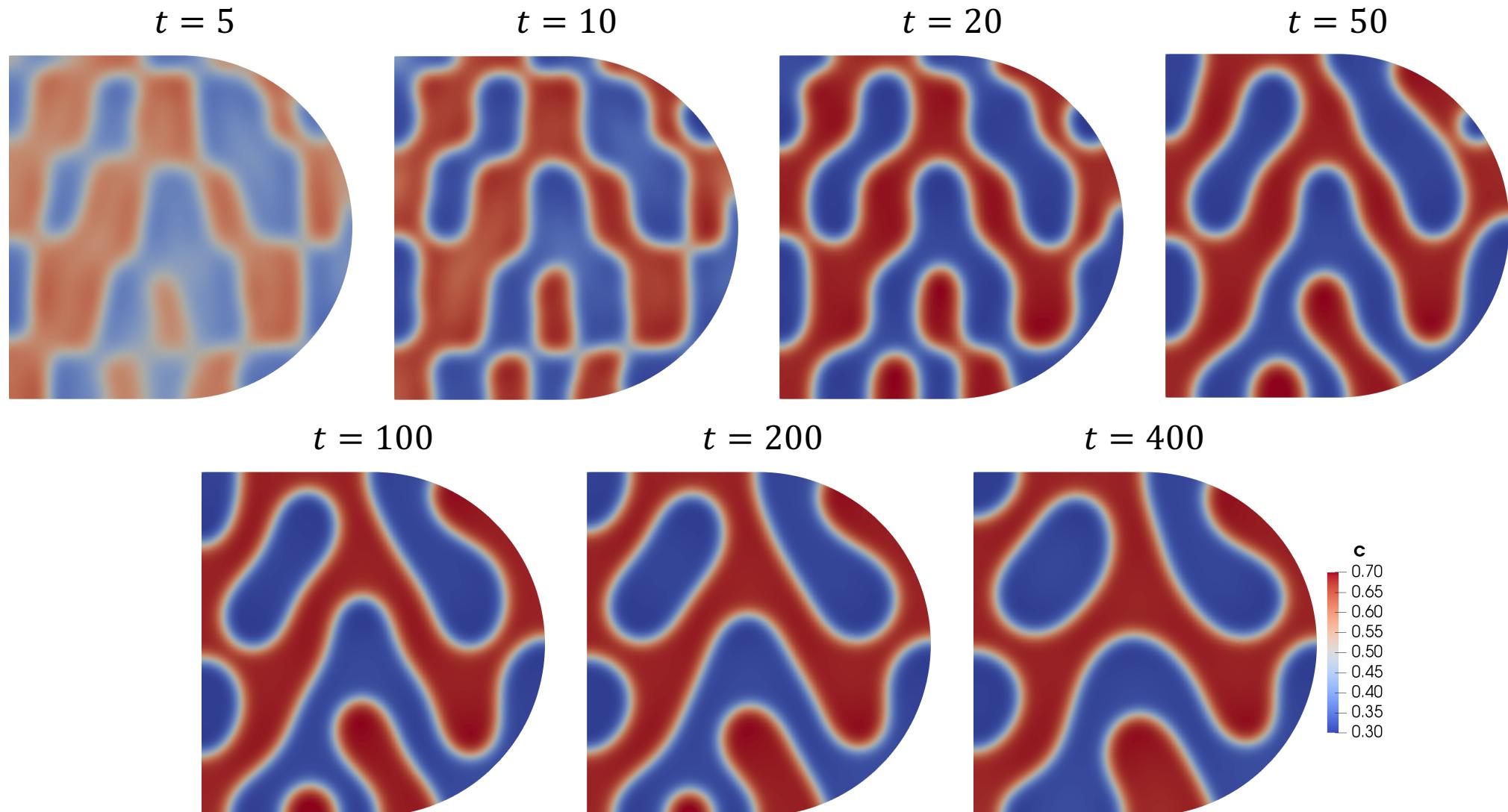
Results for (a)- Function Neumann B.C. total free energy



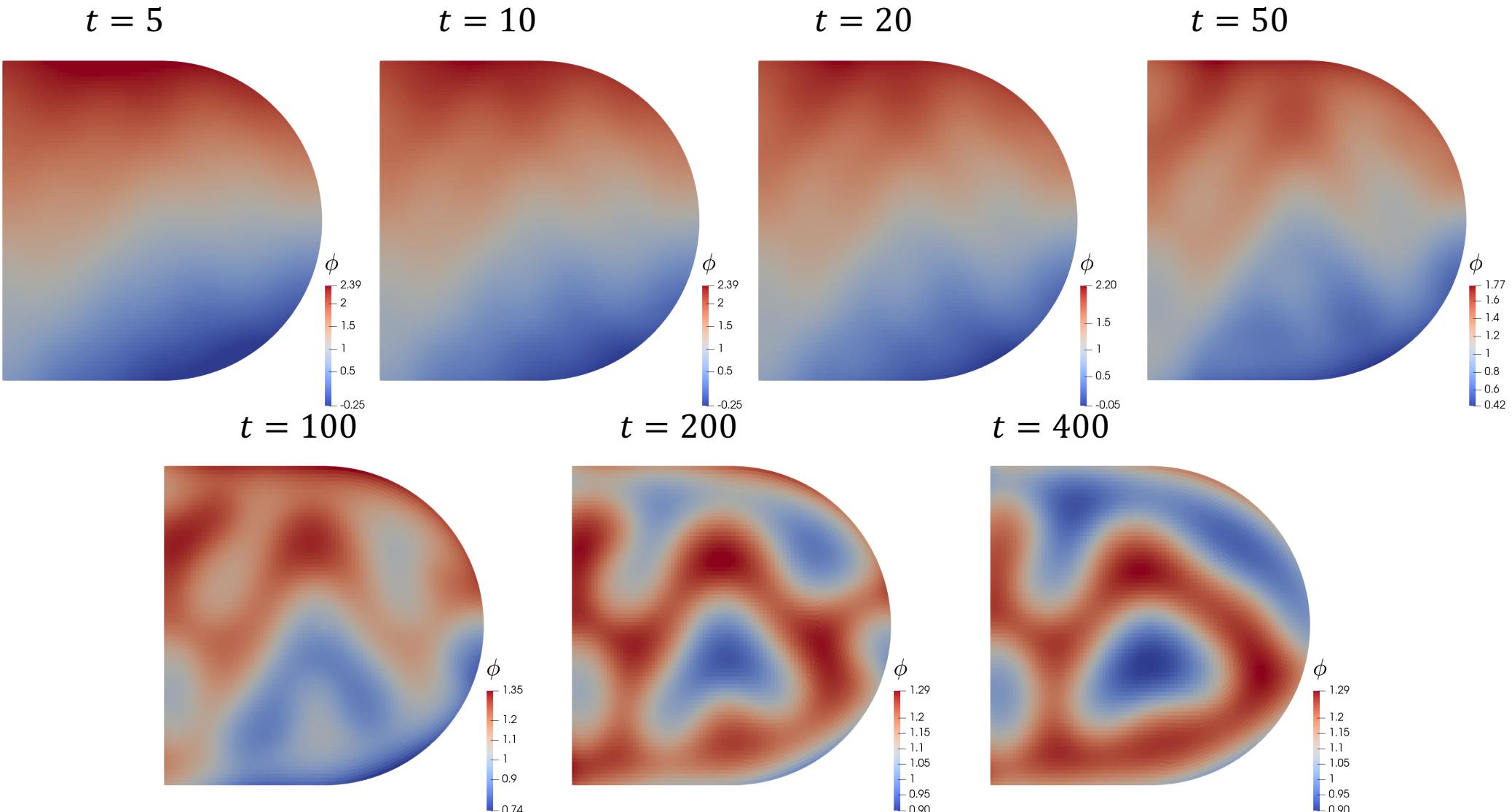
Results for (b)—Neumann B.C.: concentration field



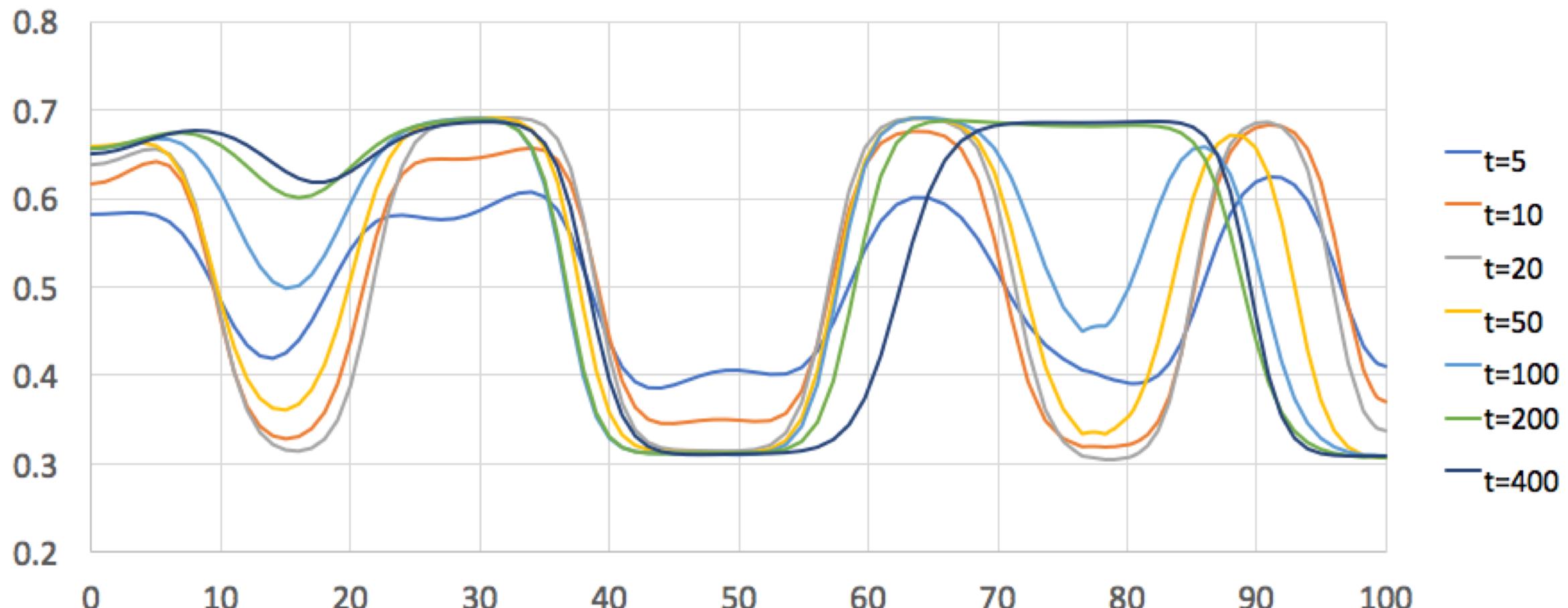
Results for (b): concentration field



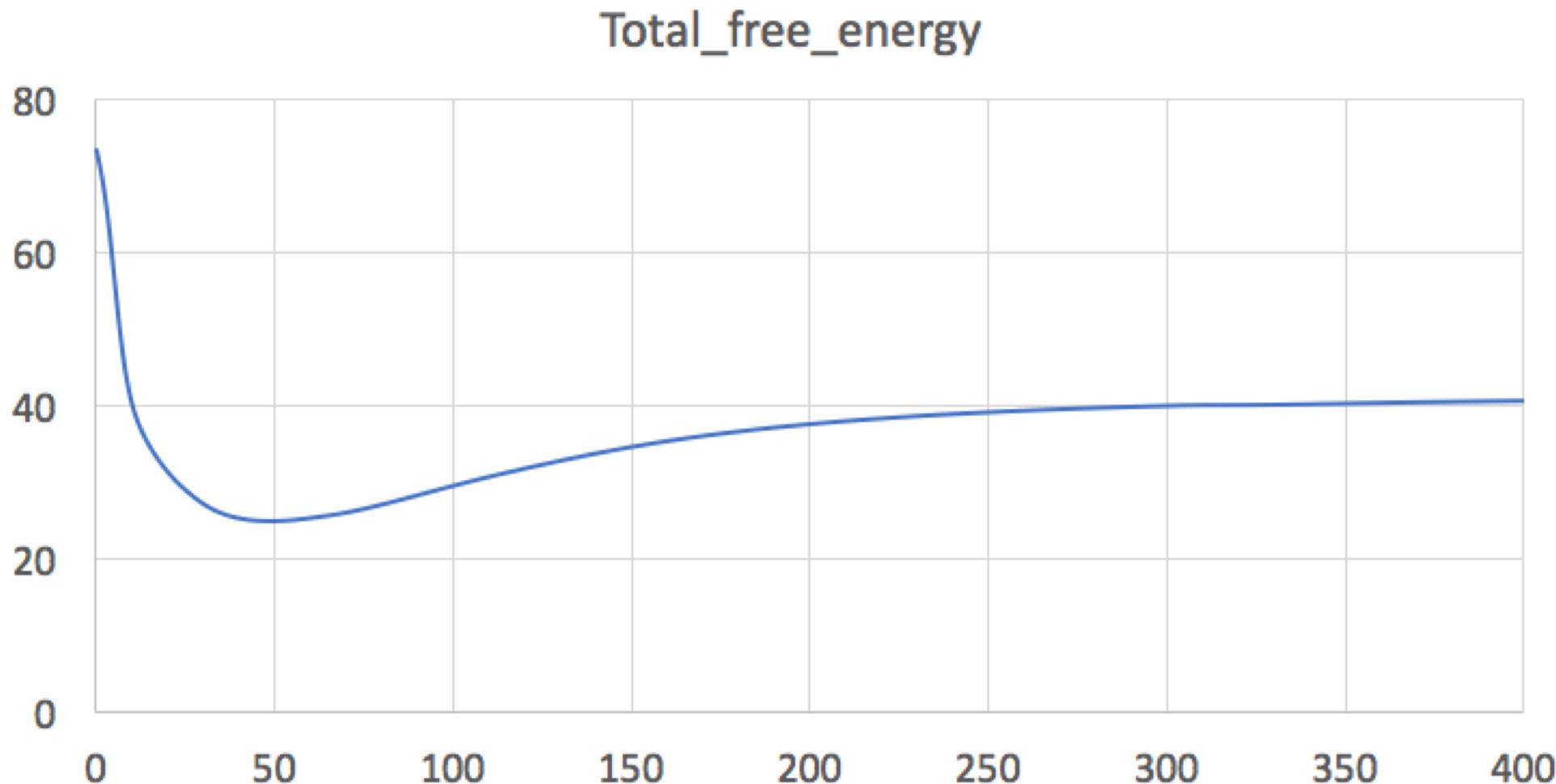
Results for (b)–Neumann B.C. Electric potential field



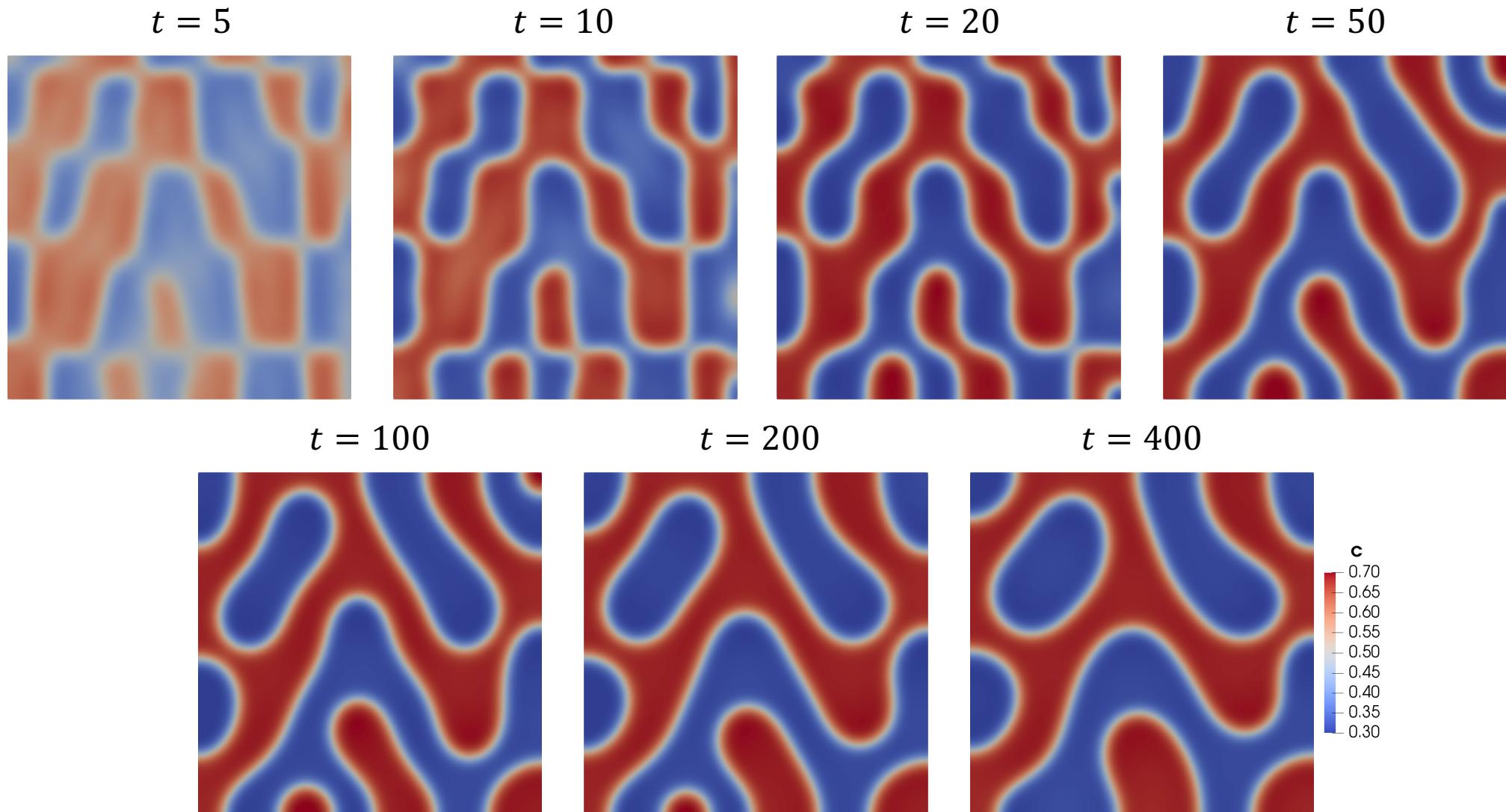
Results for (b)—Neuman B.C.: cross-sectional concentration



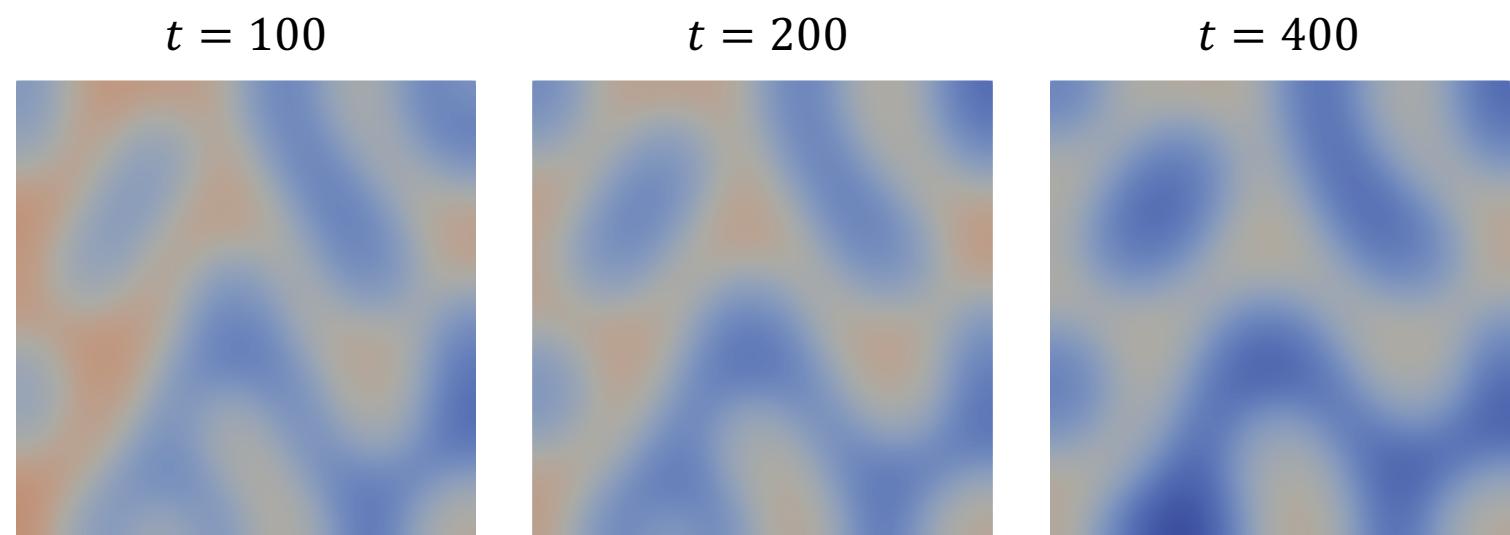
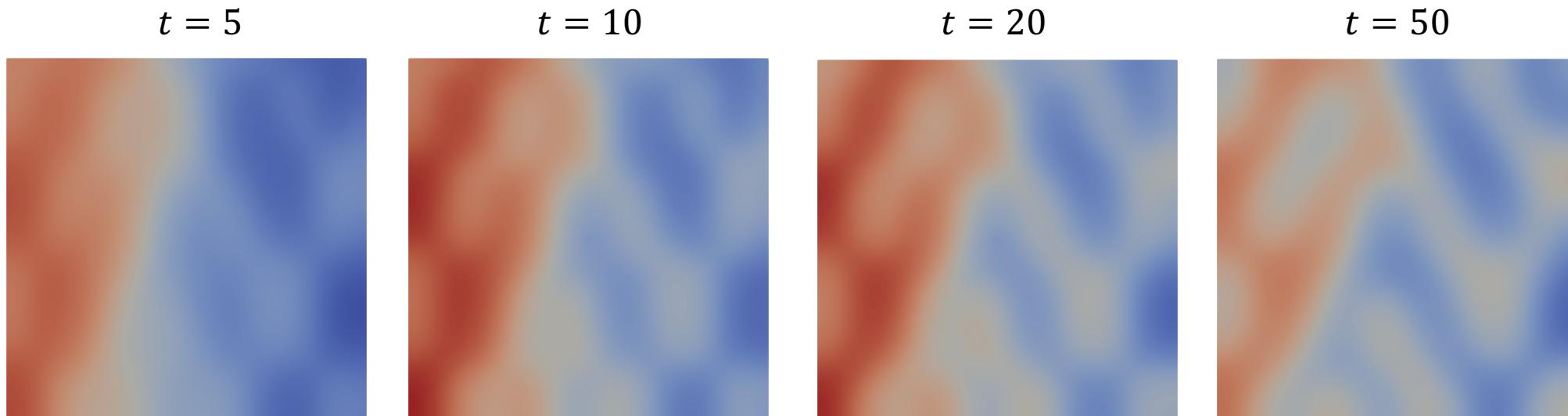
Results for (b)—Neumann B.C. total free energy



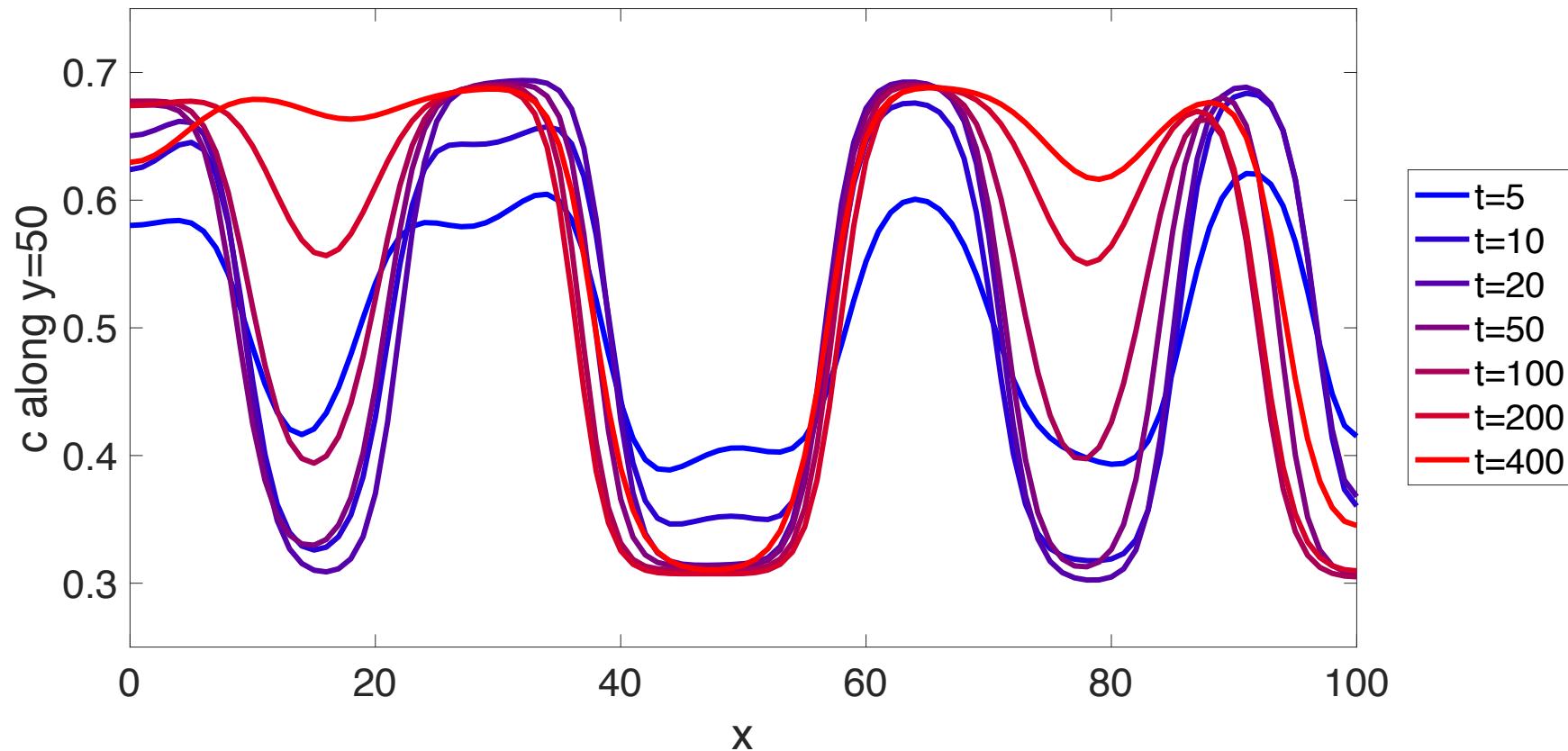
Results for (a): concentration field



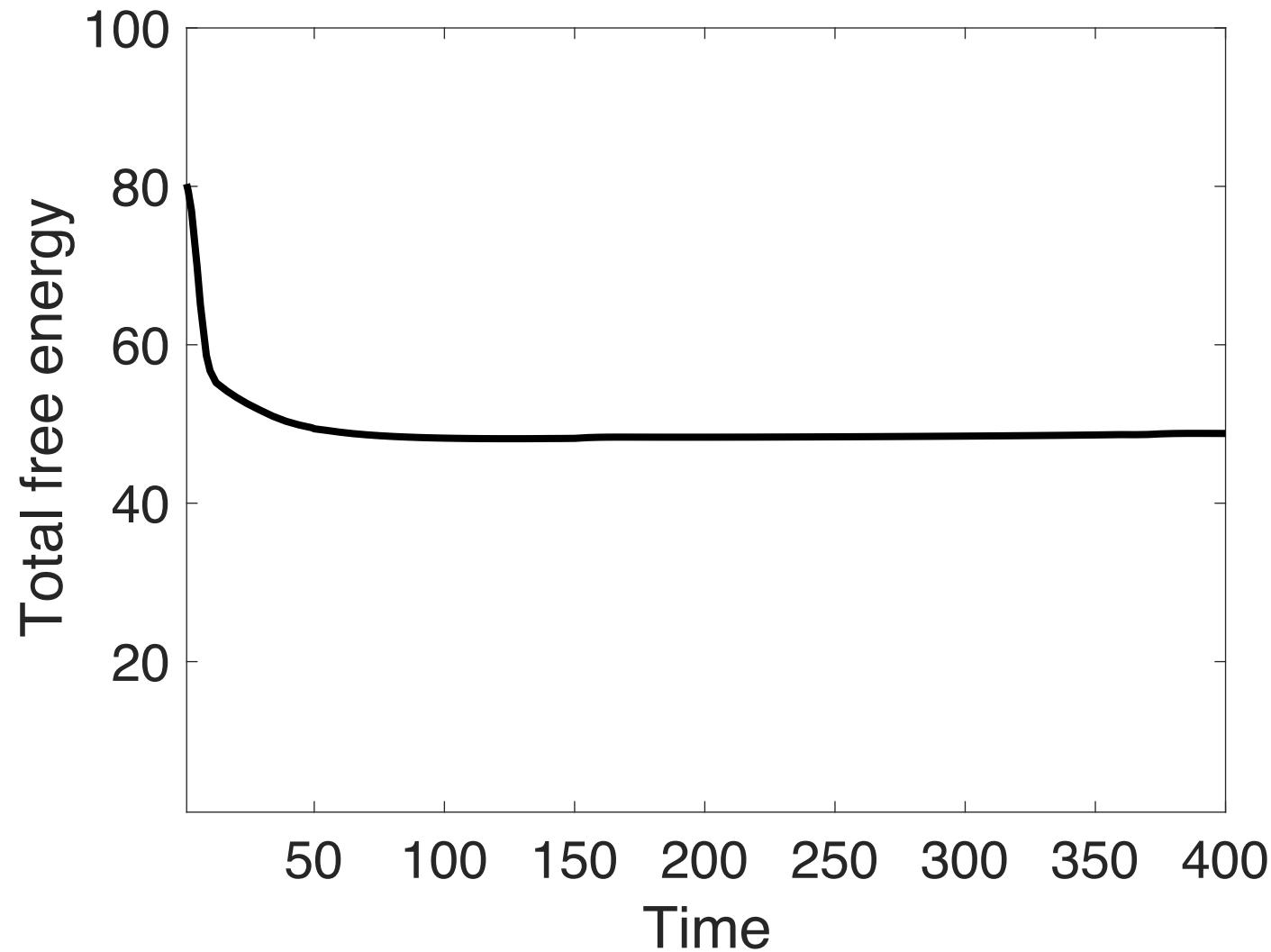
Results for (a): Electric potential field



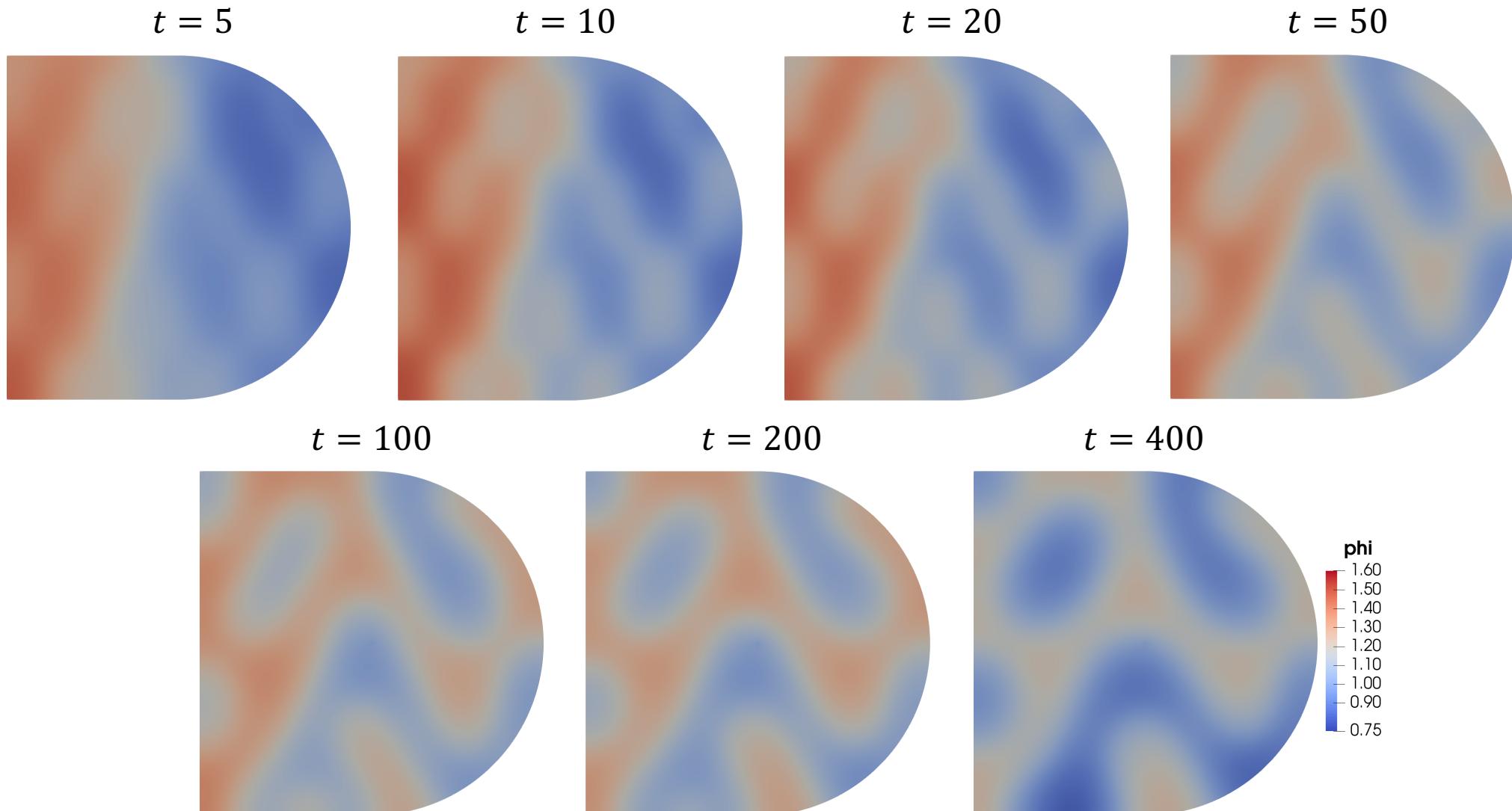
Results for (a): cross-sectional concentration



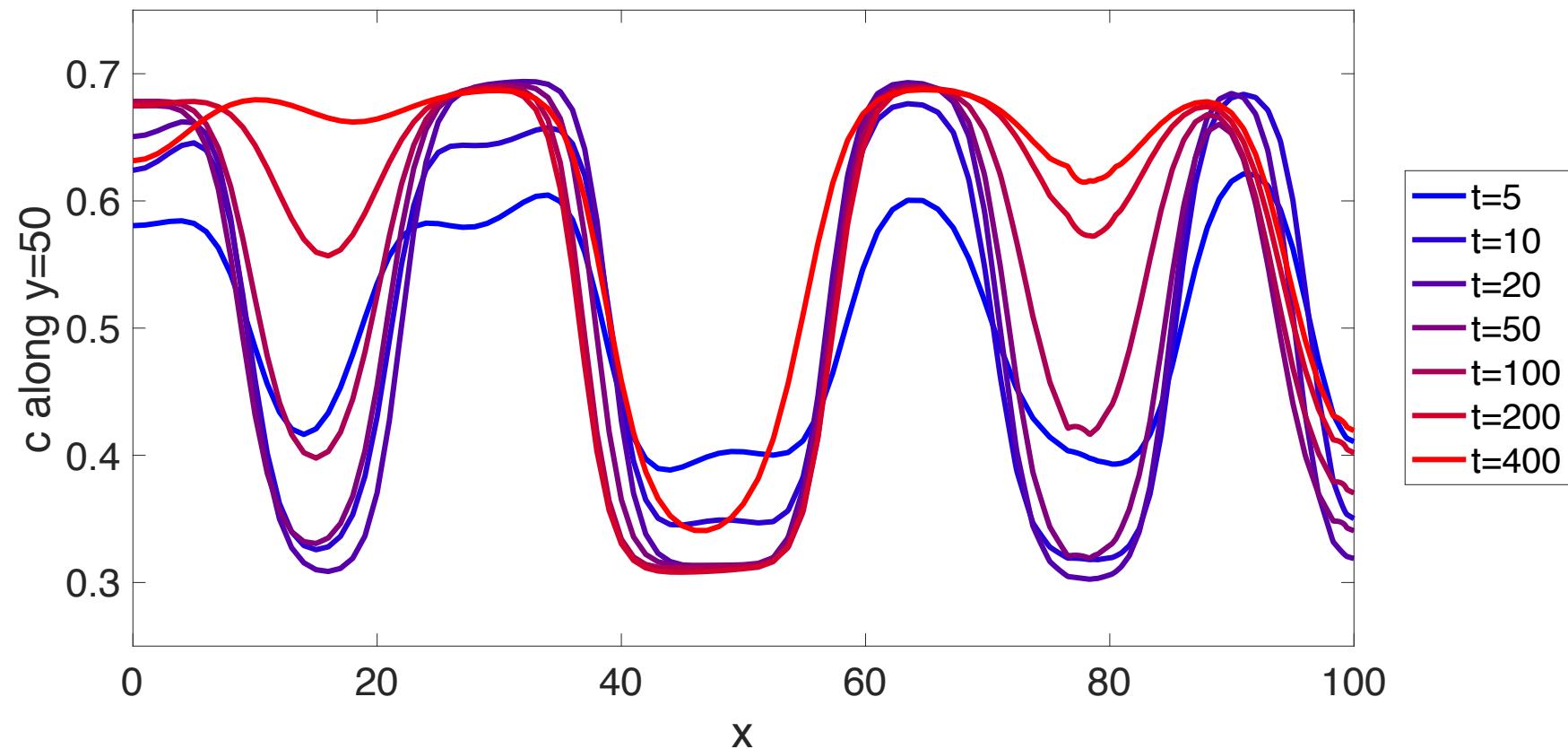
Results for (a): total free energy



Results for (b): Electric potential field



Results for (b): cross-sectional concentration



Results for (b): total free energy

