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Multiphysics Simulation of a Packed Bed Reactor

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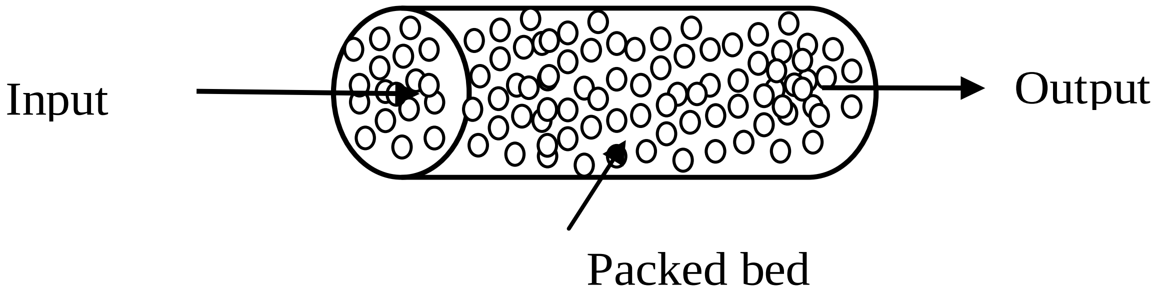
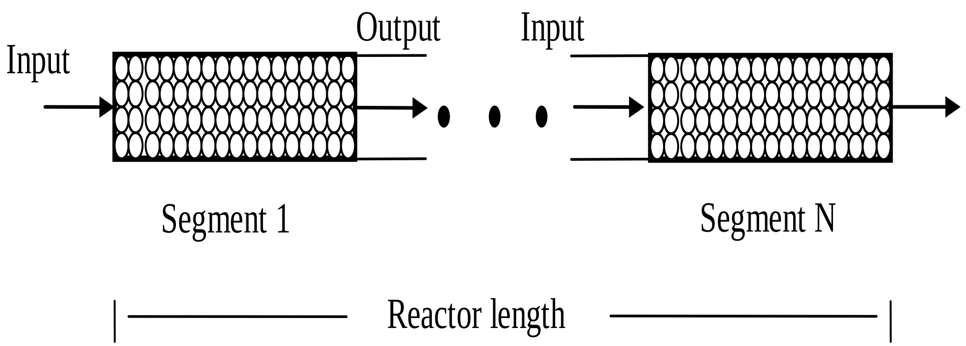
Geometry

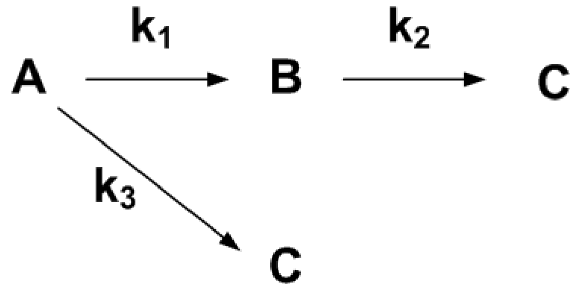
Schematic of a Packed Bed Reactor



Segmented geometry



Reaction Kinetics



A = o-xylene, B = phthalic anhydride,
C = carbon monoxide and carbon dioxide
k_i, i=1, 2, 3, = rate constants

$$r_1 = \rho_b y_o y_{Ao} k_1 (1 - x_A)$$
$$r_2 = \rho_b y_o y_{Ao} k_2 x_B$$
$$r_3 = \rho_b y_o y_{Ao} k_3 (1 - x_A)$$

Kinetics

Kinetics Parametres

(Lerou and Froment,, *Chem. Eng. Science*, vol. 32, 1977)

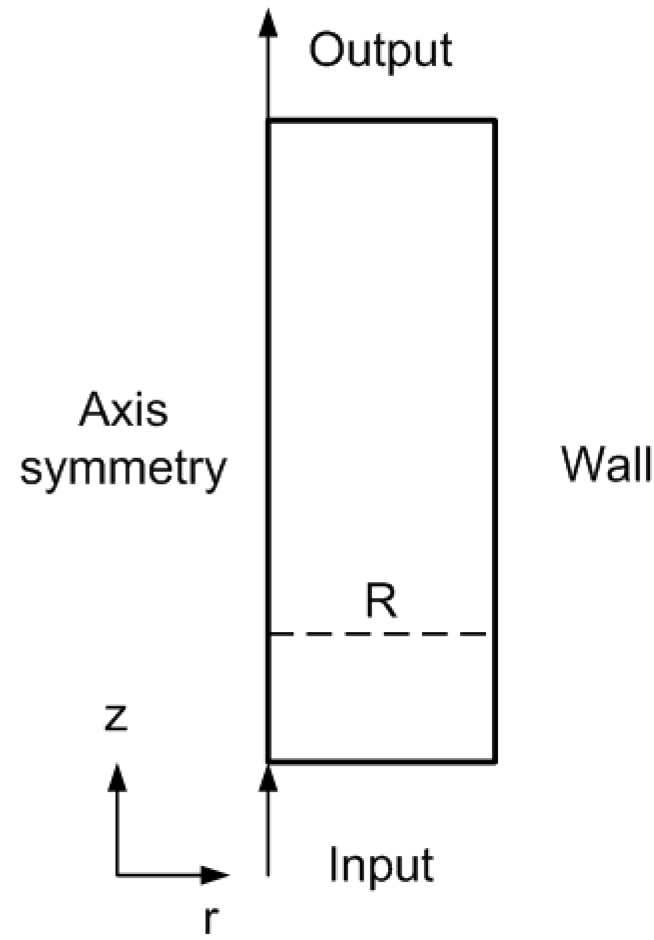
$$k_i = A_i \exp\left(-\frac{B_i}{T}\right), \quad (i = 1, 2, 3)$$

A_1 = exp(19.837) kmol/kg h
A_2 = exp(20.86) kmol/kg h
A_3 = exp(18.97) kmol/kg h
B_1 = 13588 K
B_2 = 15803 K
B_3 = 14394 K

$\Delta H_1 = -1.285 \times 10^6$ J/mol
$\Delta H_2 = -3.276 \times 10^6$ J/mol
$\Delta H_3 = \Delta H_1 + \Delta H_2$

Lumped Model

Lumped Model



Mass-Energy Balance

$$\nabla \cdot \left(-D_{eff} \nabla x_i + u_s x_i\right) = \frac{1}{c_{tot} y_{Ao}}$$

$$u_s \rho_g C_p \nabla \cdot T - \nabla \cdot \left(-k_{eff} \nabla T\right) = \sum_{i=1}^{3} (-\Delta H_i) r_i$$

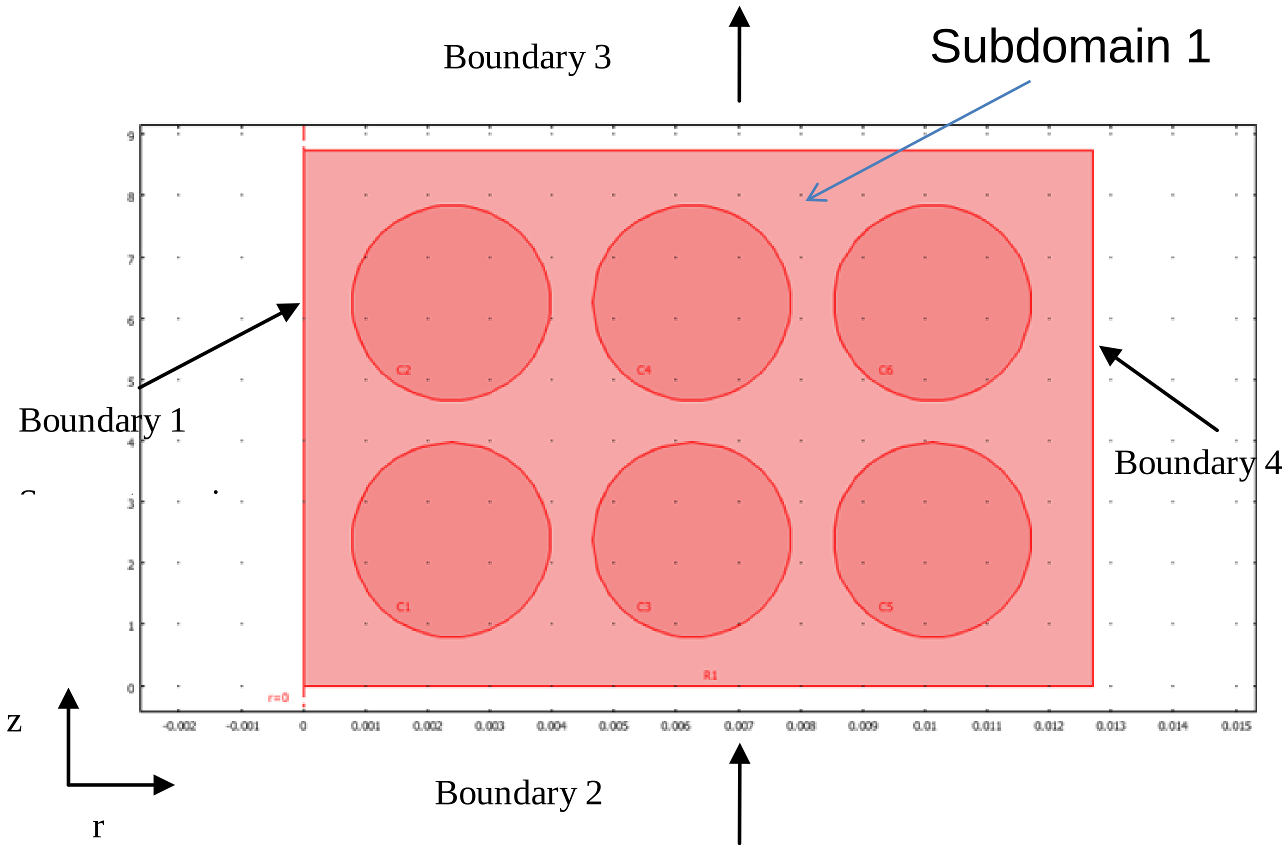
Boundary Conditions

$$\frac{\partial x_B}{\partial r}(0,z) = \frac{\partial x_C}{\partial r}(0,z) = 0, \frac{\partial T}{\partial r}(0,z) = 0$$

$$\frac{\partial x_B}{\partial r}(R,z) = \frac{\partial x_C}{\partial r}(R,z) = 0, k_{eff} \frac{\partial T}{\partial r}(R,z) = -\alpha(T - T_c)$$

Model

Segment Model



Length = 0.00873 m, radius = 0.0127 m, circle radius = 0.00159 m, uniform separation = 0.00079 m

Application Modes

Navier-Stokes equations - Subdomain 1

$$\rho_g u \cdot \nabla u = \nabla \cdot [-pI + \mu(\nabla u + (\nabla u)^T)]$$

$$\nabla \cdot u = 0$$

Initial conditions $\begin{cases} u_{to} = 0 \\ v_{to} = 0 \\ p_{to} = p_o \end{cases}$

Convection and diffusion equations

Subdomain 1

$$\nabla \cdot (-D\nabla c_B) = -u \cdot \nabla c_B, u = [u\ v]^T$$

$$\nabla \cdot (-D\nabla c_C) = -u \cdot \nabla c_C, u = [u\ v]^T$$

Subdomains 2, .., 7 (circles)

$$\nabla \cdot \left(-D_{eff}\nabla c_B\right) = r_B / y_{Ao}$$

$$\nabla \cdot \left(-D_{eff}\nabla c_C\right) = r_C / y_{Ao}$$

Initial conditions $c_{Bto} = 0, c_{Cto} = 0$

Energy balance equations

Subdomain 1

$$\nabla \cdot (-k \cdot \nabla T) = -\rho_g C_{pg} u \cdot \nabla T;$$

$$u = [u\ v]$$

Subdomains 2, .., 7 (circles)

$$\nabla \cdot \left(-k_{eff} \cdot \nabla T\right) = (-\Delta H_1) r_B + (-\Delta H_2) r_C - \rho_g C_p u \cdot \nabla T$$

Initial condition $T_{to} = T_0$

BCs / Navier-Stokes equations

Outlet

$$p_{bo} = p_o$$
$$\mu(\nabla u + (\nabla u)^T)n = 0$$

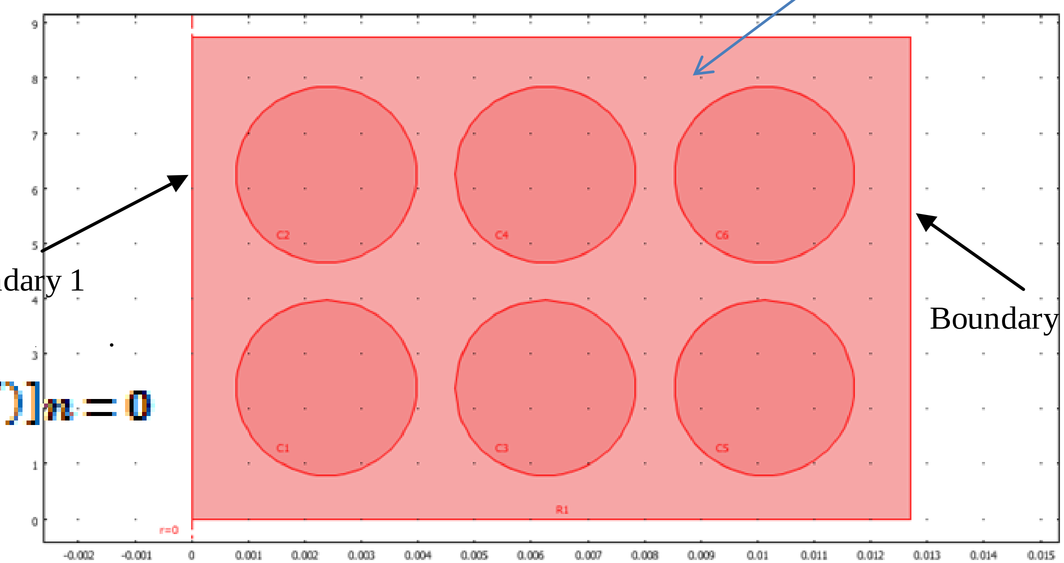
Boundary 3

Subdomain 1

Symmetry

Boundary 1

$$n \cdot u = 0$$
$$t \cdot [-pI + \mu(\nabla u + (\nabla u)^T)]n = 0$$



No slip

Boundary 4

$$u = 0$$

z

r

Boundary 2

Inlet / Segment 1

$$\begin{cases} u_o = 0 \\ v_o = u_s \end{cases}$$

Other segments

$$\begin{cases} u_o = u_{prev} \\ v_o = v_{prev} \end{cases}$$

BCs / Convection and diffusion equations

Convective flux

$$\mathbf{n}\cdot(-D\nabla c_B)=0$$
$$\mathbf{n}\cdot(-D\nabla c_C)=0$$

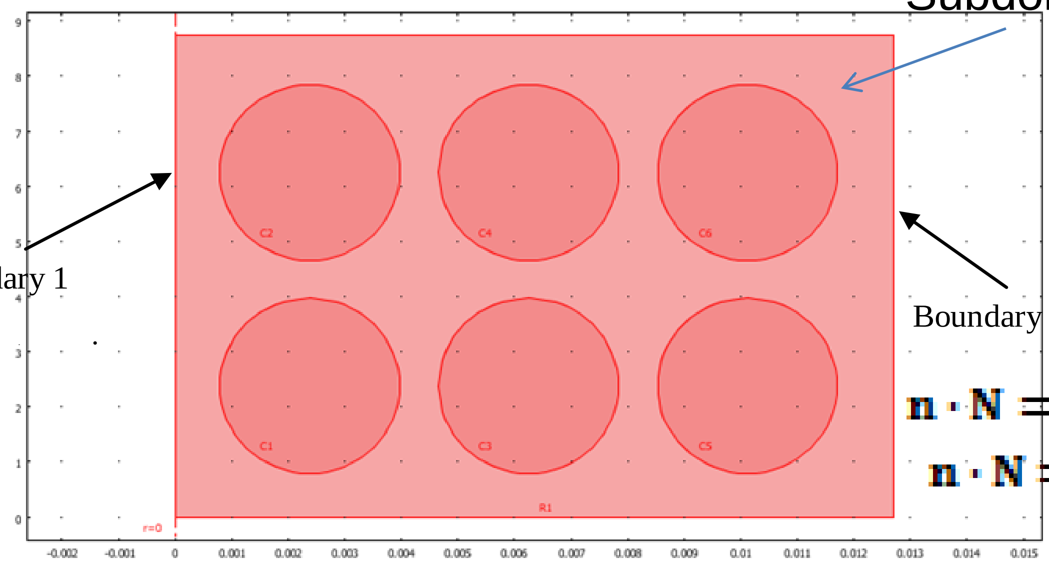
Boundary 3

Subdomain 1

Symmetry

$$r=0$$

Boundary 1



Boundary 4

Insulation

$$\mathbf{n}\cdot\mathbf{N}=0, \mathbf{N}=-D_{eff}\nabla c_B+c_B u,$$
$$\mathbf{n}\cdot\mathbf{N}=0, \mathbf{N}=-D_{eff}\nabla c_B+c_B u$$

z

r

Boundary 2

Inlet / Segment 1 $c_{Bo}=0, c_{Co}=0,$

Other segments $c_{Bo}=c_{B,prev}, c_{Co}=c_{C,prev}$

BCs / Energy balance equations

Convective flux $\mathbf{n}\cdot(-k\cdot\nabla T)=0$

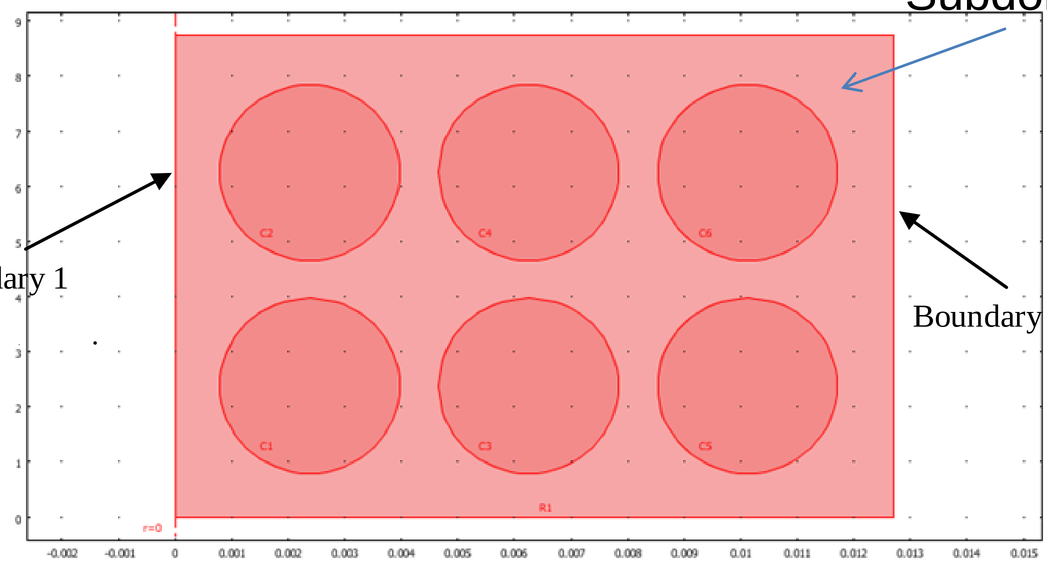
Boundary 3

Subdomain 1

Symmetry

$r=0$

Boundary 1



Boundary 4

Heat flux

$$\mathbf{n}\cdot\mathbf{q}=-\alpha(T-T_0)$$
$$\mathbf{q}=-k\cdot\nabla T+\rho_0 C_{p0}T\mathbf{u}$$

z

r

Boundary 2

Inlet / Segment 1 $T_{to}=T_0$

Other segments $T_{to}=T_{prev}$

$\boxed{u_{prev}\,,\, v_{prev}\,,\, c_{B,prev}\,,\, c_{B,prev}\,,\, T_{prev}\ =}$ $\tilde{\varphi}_i=\dfrac{2}{R^2}\displaystyle\int_0^R \varphi_i(r)r\,dr$

Approach

Approach

a. First set up the 2D-axis-symmtry geometry and application modes.

b. Mesh generation by selecting a maximum element size of 1×10^{-4} m for boundaries 1, 2, 3 and 4, and 0.5×10^{-5} for interior circle boundaries.

c. Next set up subdomains 1 and subdomains 2-6 for the different application modes and boundary conditions.

d. Now solve the problem. First choose the Navier-Stokes equations to compute the velocity components (u, v) for subdomain 1. Then save variables and solve energy and mass balance equations.

e. Save the above process as a matlab file and modify it for the successive changes in boundary and input conditions of each reactor segment.

f. Execution of the matlab file and analysis of results under.

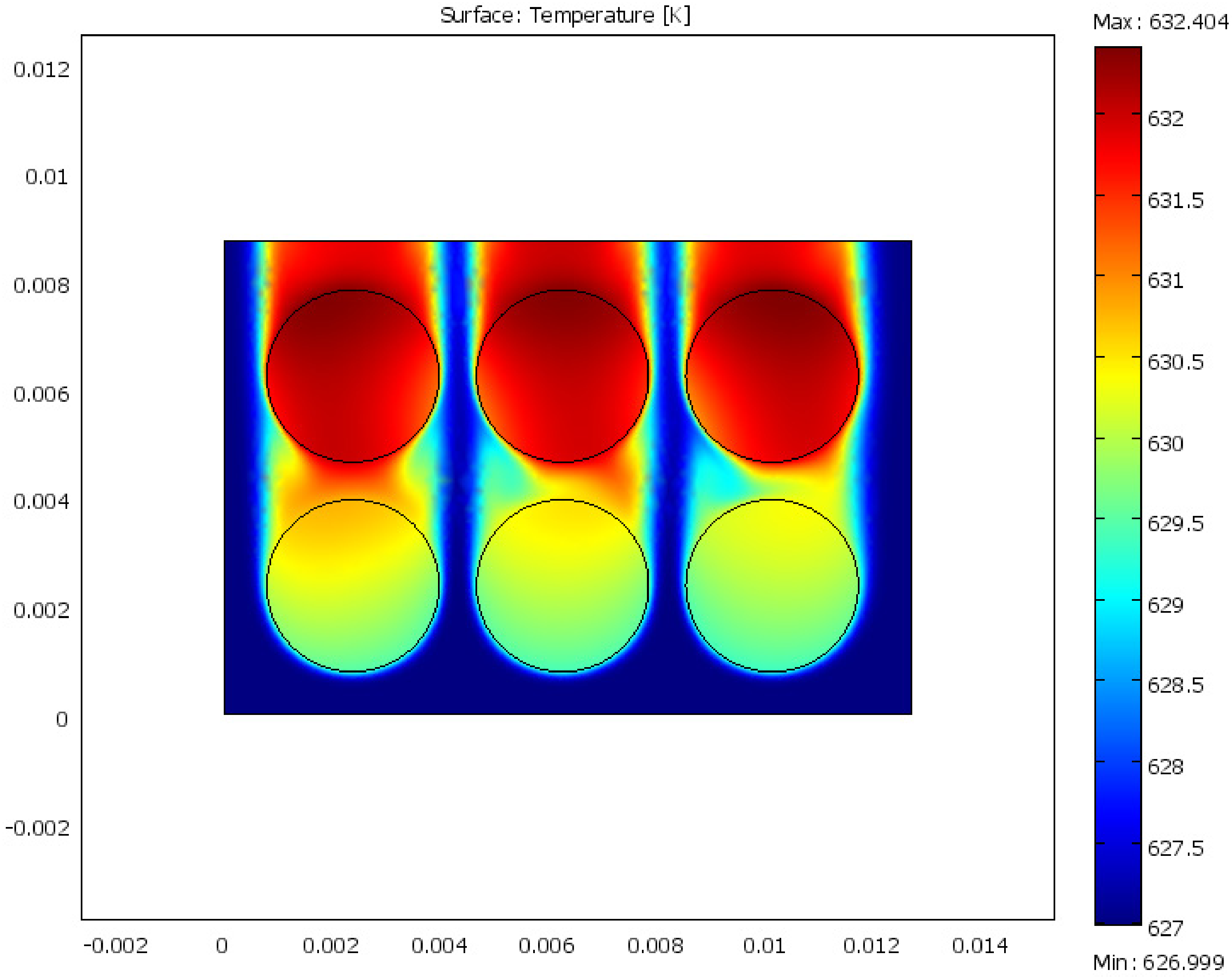
Results

Model Parameters

Reactor radius, R = 1.27 cm,
Superficial velocity, v_s = 1.064 m/s, (m/s),
Inlet temperature, T_0 = 627 K,
Pressure, $p_o = 1.013x10^5$ Pa
Inlet total concentration, c_{tot} = 44.85 mol/m^3 mol/m,
Inlet mole fraction of o-xylene, y_{Ao} = 0.00924,
Inlet mole fraction of oxygen, y_0 = 0.208,
Catalyst bulk density ρ_b = 1300 kg/m^3,
Gas density ρ_g = 1293 kg/m^3,
Gas heat capacity C_p = 1046 J/(kg K),
Heat transfer coefficient α = 156 W/(m^2 K).
Effective diffusion constant, D_{eff} = 3.19e-7 m^2/s,
Diffusivity of xylene in air, D = 8.074x10^{-5} m^2/s,
Effective thermal conductivity, k_{eff} = 0.779 W/(m K),
Gas thermal conductivity, k = 0.0318 W/(m K).

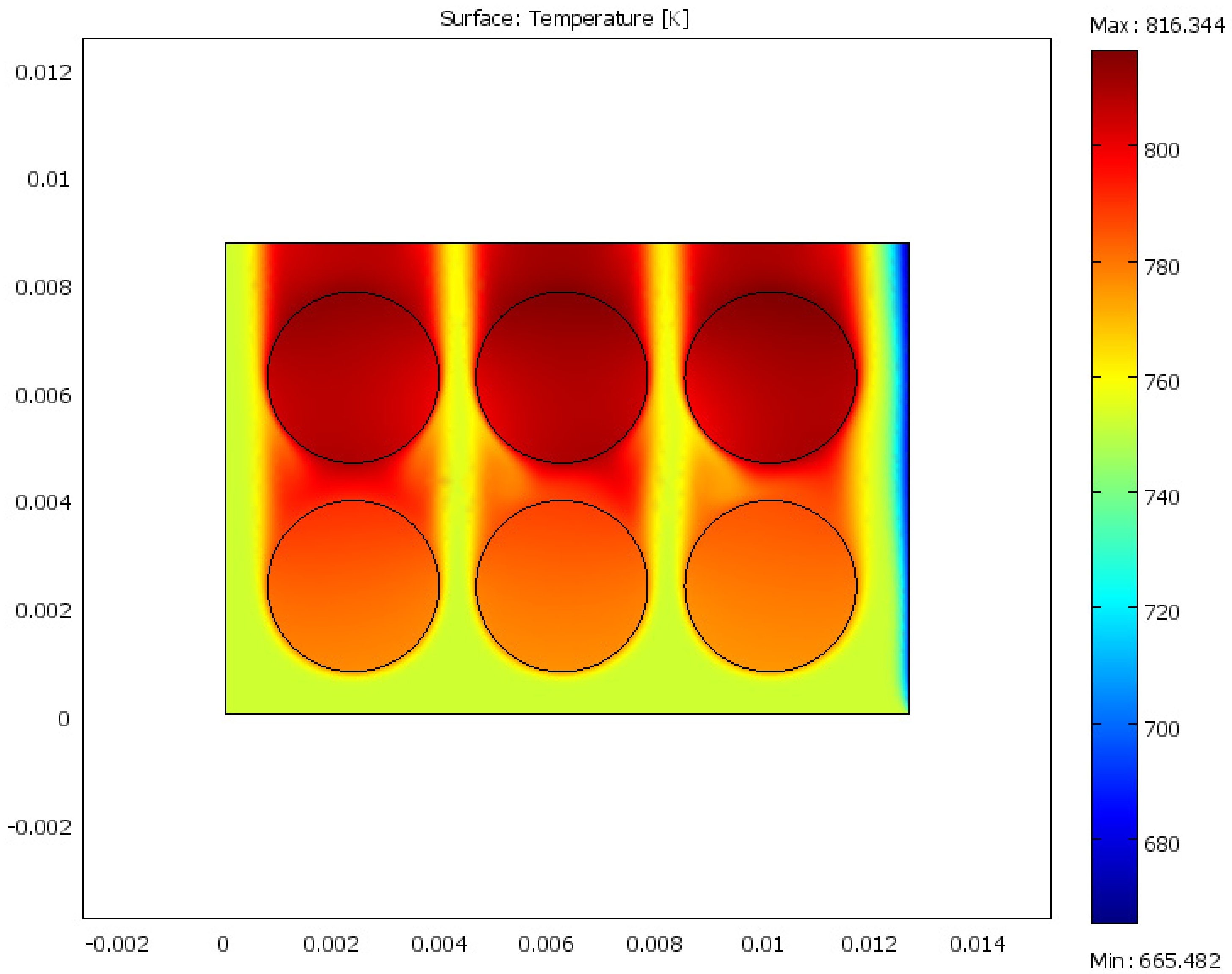
Results

Temperature distribution, segment 1, L = 0.0873 m



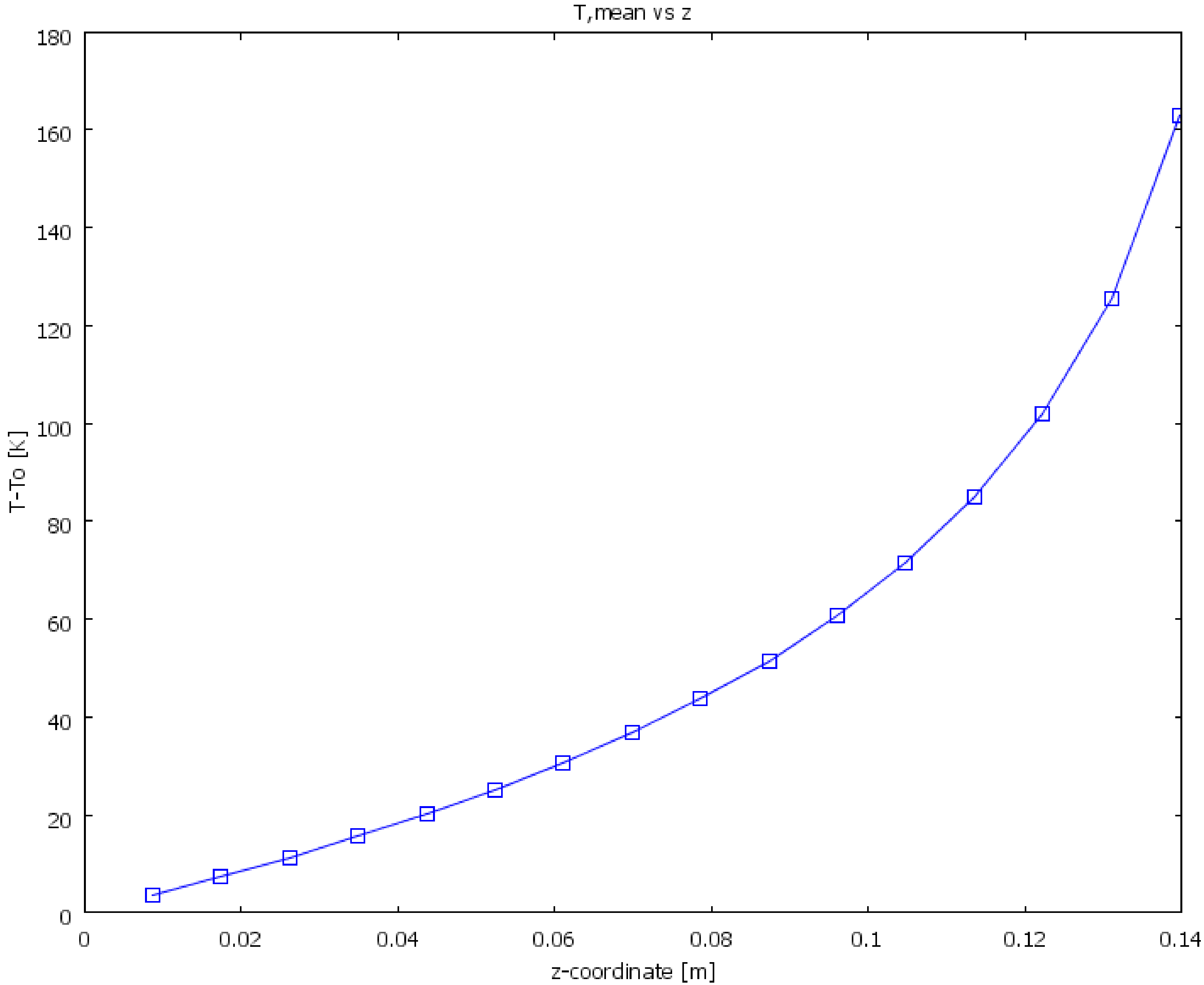
Results

Temperature distribution, segment 16, *L* = *L* = 0.13968 m



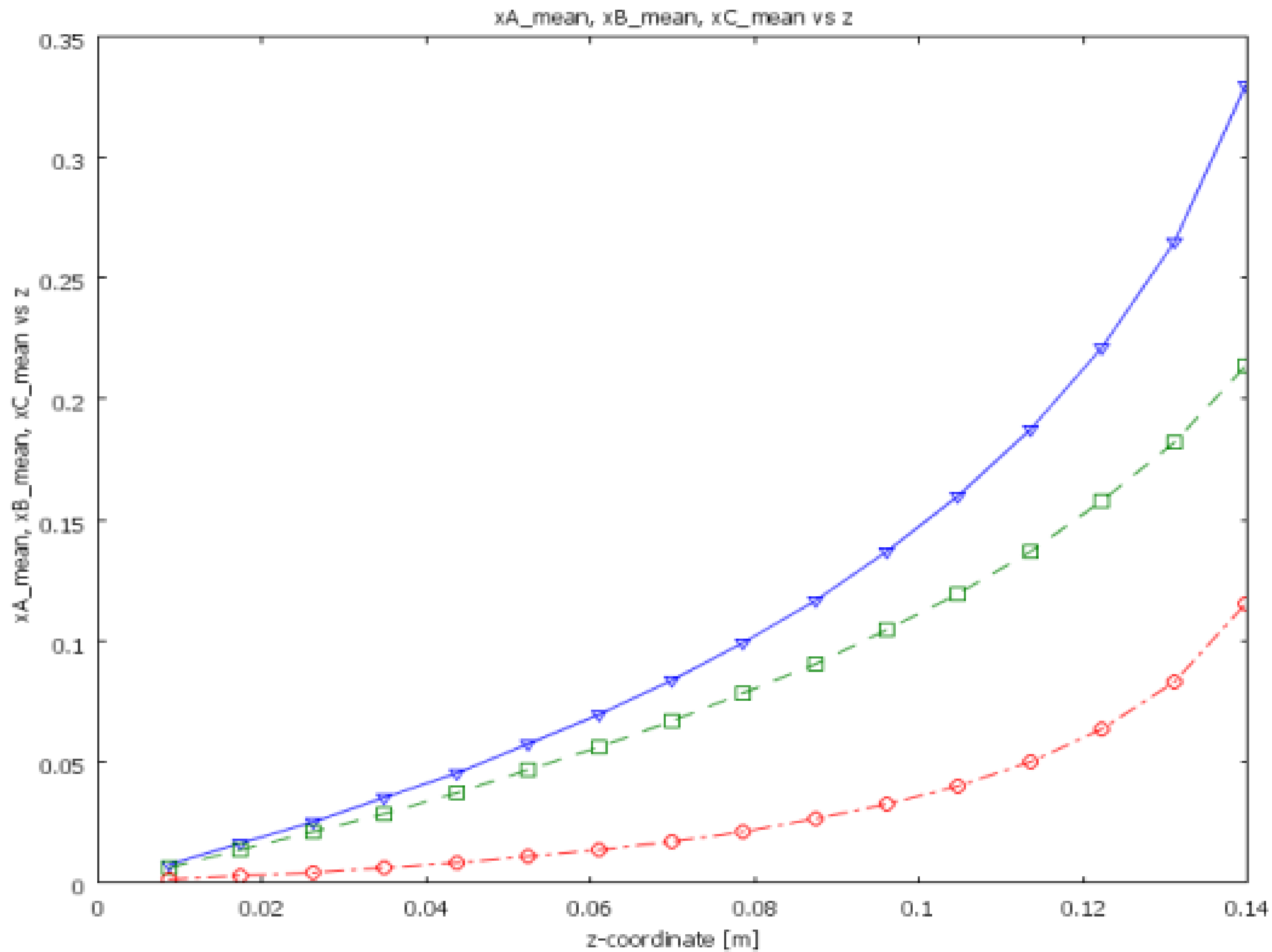
Average temperature profile, *L* = 0.13968 m

Results

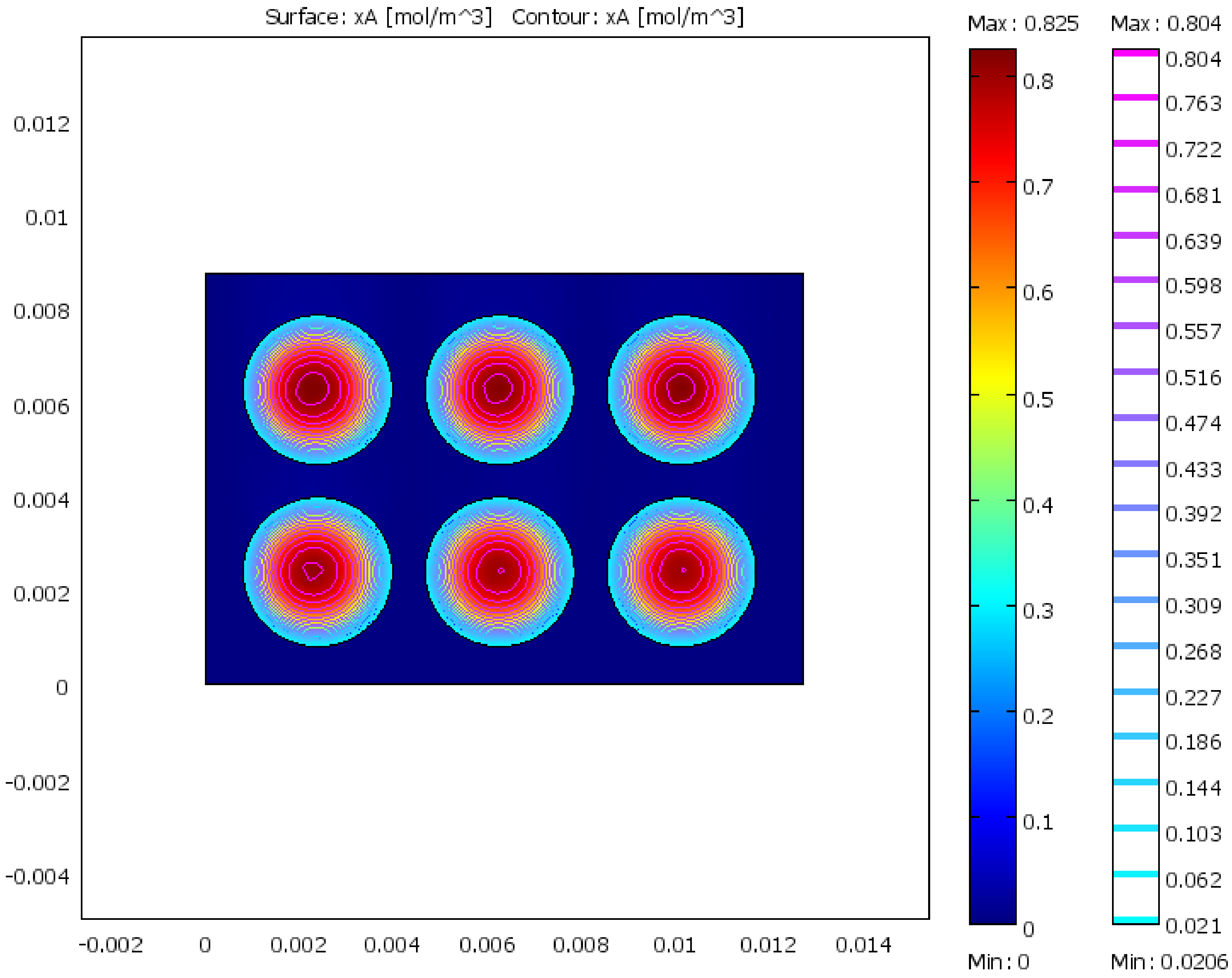


Results

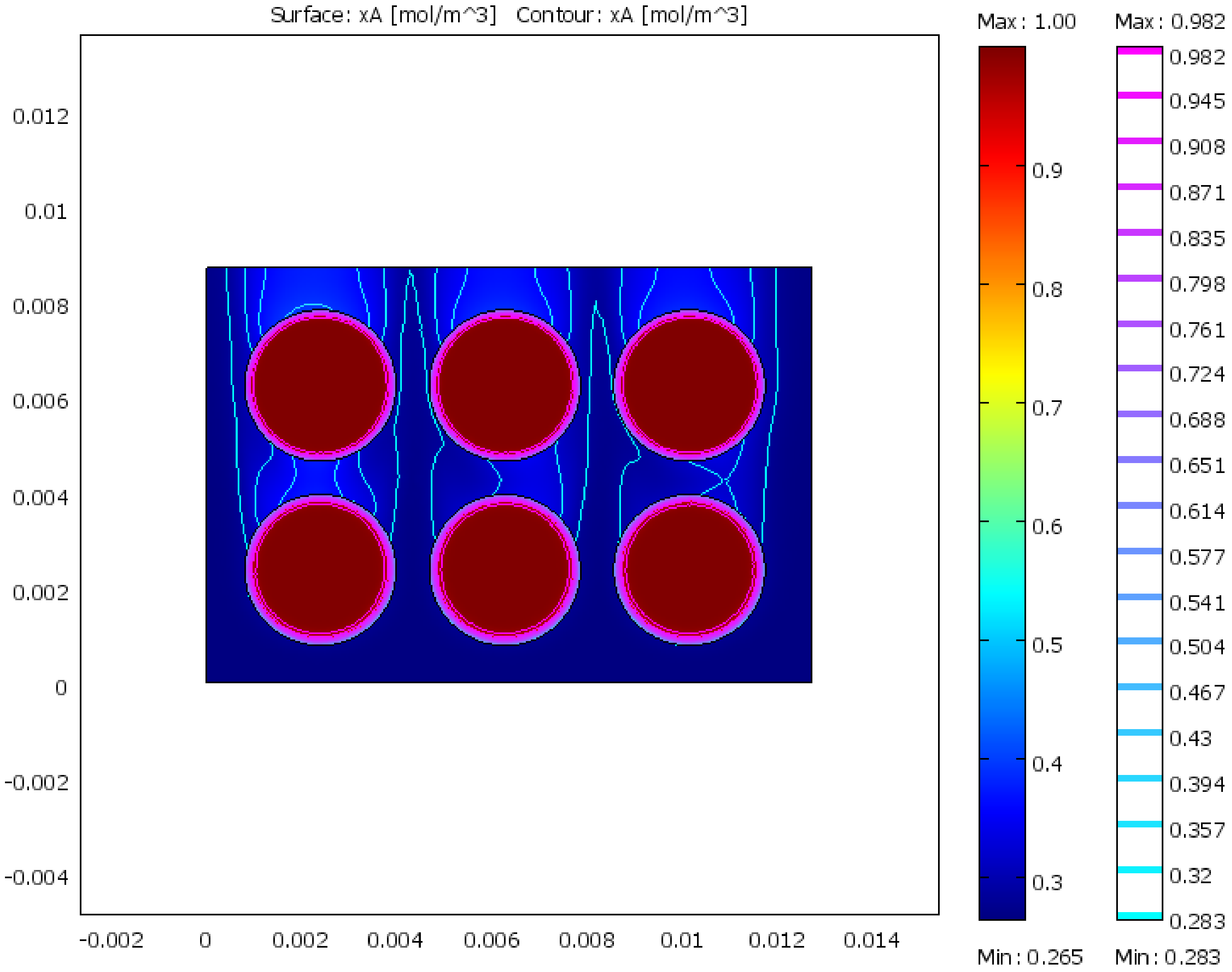
Average conversions, *L* = 0.13968 m



Conversion of *A*, segment 1, *L* = 0.0873 m



Conversion of *A*, segment 16, *L* = 0.13968 m



Conclusion

High temperatures increases or hot-spots occurred near reactor inlet. In order to study possible undesired conversions and catalyst damage, a more detailed model is desirable. For a future work we suggest consideration of a geometry model with intra pellet gaps and in contact with each other for the packed bed reactor simulation. This study should include sensitivity analysis of inlet temperature and heat transfer through the wall.

Many Thanks