BT209

Bioreaction Engineering

20/04/2023

Tutorial: Heterogeneous reaction

Problem 1

EX-1: Suspended cells form spherical aggregates approximately 1.5 mm in diameter. Medium is recirculated with a superficial liquid velocity of 0.83 cm/s. At a bulk concentration of 8 mg/L, oxygen is consumed at a rate of 0.28 mg per g wet weight of cells per hour. Assume that the density and viscosity of the medium are similar to water and the specific gravity of wet cells is 1. The effective diffusivity of oxygen in the aggregates is 9 X 10^{-6} cm^2/S, or half that in the medium. Oxygen uptake follows zero-order kinetics.

(a) Does external mass transfer affect the oxygen uptake rate?

(b) Roughly, what would you expect the profile of oxygen concentration to be within the aggregates?

Use the following relationship for external mass transfer coefficient

$$Sh = 2 + 0.6\, Re_p^{0.5}\, Sc^{0.33}$$

Correlations for k_S are expressed using the following dimensionless groups:

$$Re_p = \text{(particle) Reynolds number} = \frac{D_p\, u_{pL}\, \rho_L}{\mu_L}$$

$$Sc = \text{Schmidt number} = \frac{\mu_L}{\rho_L\, \mathscr{D}_{AL}}$$

$$Sh = \text{Sherwood number} = \frac{k_S D_p}{\mathscr{D}_{AL}}$$

$$Gr = \text{Grashof number} = \frac{g\, D_p^3\, \rho_L\, (\rho_p - \rho_L)}{\mu_L^2}$$

D_p is the particle diameter, u_{pL} is the linear velocity of the particle relative to the bulk liquid, ρ_L is liquid density, μ_L is liquid viscosity, $\mathscr{D}_{AL}$ is the molecular diffusivity of component A in the liquid, k_S is the liquid–solid mass transfer coefficient, g is gravitational acceleration, and ρ_p is the particle density. The Sherwood number contains the mass transfer coefficient and represents the ratio of overall mass transfer rate to diffusive mass transfer rate through the boundary layer. The Schmidt number represents the ratio of momentum diffusivity to mass diffusivity and is evaluated from the physical properties of the system. At constant temperature, pressure, and composition, *Sc* is constant for Newtonian fluids. The Grashof number represents the ratio of gravitational forces to viscous forces and is important when the particles are neutrally buoyant. The form of the correlation used to evaluate *Sh* and therefore k_S depends on the configuration of the mass transfer system, the flow conditions, and other factors.

Solution

a)

$$\boxed{\frac{C_{As}}{C_{Ab}} = 1 - \frac{V_p}{S_x}\frac{r_{A,obs}}{k_S\,C_{Ab}}}$$

VP/Sx for spherical particle=R/3

$$Sh = 2 + 0.6\,Re_p^{0.5}\,Sc^{0.33}$$

$$Sc = \text{Schmidt number} = \frac{\mu_L}{\rho_L\,\mathscr{D}_{AL}}$$ =556

$$Re_p = \text{(particle) Reynolds number} = \frac{D_p\,u_{pL}\,\rho_L}{\mu_L}$$ =12.5

$$Sh = \text{Sherwood number} = \frac{k_S D_p}{\mathscr{D}_{AL}}$$ =kS x 0.0015/9x 10^-10

k_S =1.44 x 10^{-5} m/s (external mass transfer coefficient)

CAS/Cab=0.83

Therefore external mass transfer is present but very small

b)

$$\boxed{R_{max} = \sqrt{\frac{6\mathscr{D}_{Ae}C_{As}}{k_0}}}$$

C_{AS}=0.83*8=6.64 g/m3

k_0 for zeroth order= rA= 0.28 mg/g cell/hr
0.0778 g/m3/s

Rmax=0.006789 m=0.679 mm

Particle diameter=1.5/2=0.75 mm

Therefore just near the center it will be zero

Problem 2

Non-viable yeast cells are immobilised in alginate beads. The beads are stirred in glucose medium under anaerobic conditions. The effective diffusivity of glucose in the beads depends on cell density according to the relationship:

$$\mathscr{D}_{Ae} = 6.33 - 7.17 y_C$$

where $\mathscr{D}_{Ae}$ is effective diffusivity $\times 10^{10}$ $m^2\ s^{-1}$ and y_C is the weight fraction of yeast in the gel. Rate of glucose uptake can be assumed to be zero order; the rate constant at a yeast density in alginate of 15 wt% is 0.5 g l^{-1} min^{-1}. For maximum reaction rate, the concentration of glucose inside the particles should remain above zero.

(a) Plot the maximum allowable particle size as a function of bulk glucose concentration between 5 g l^{-1} and 60 g l^{-1}.
(b) For 30 g l^{-1} glucose, plot R_{max} as a function of cell loading between 10 and 45 wt%.

Solution:

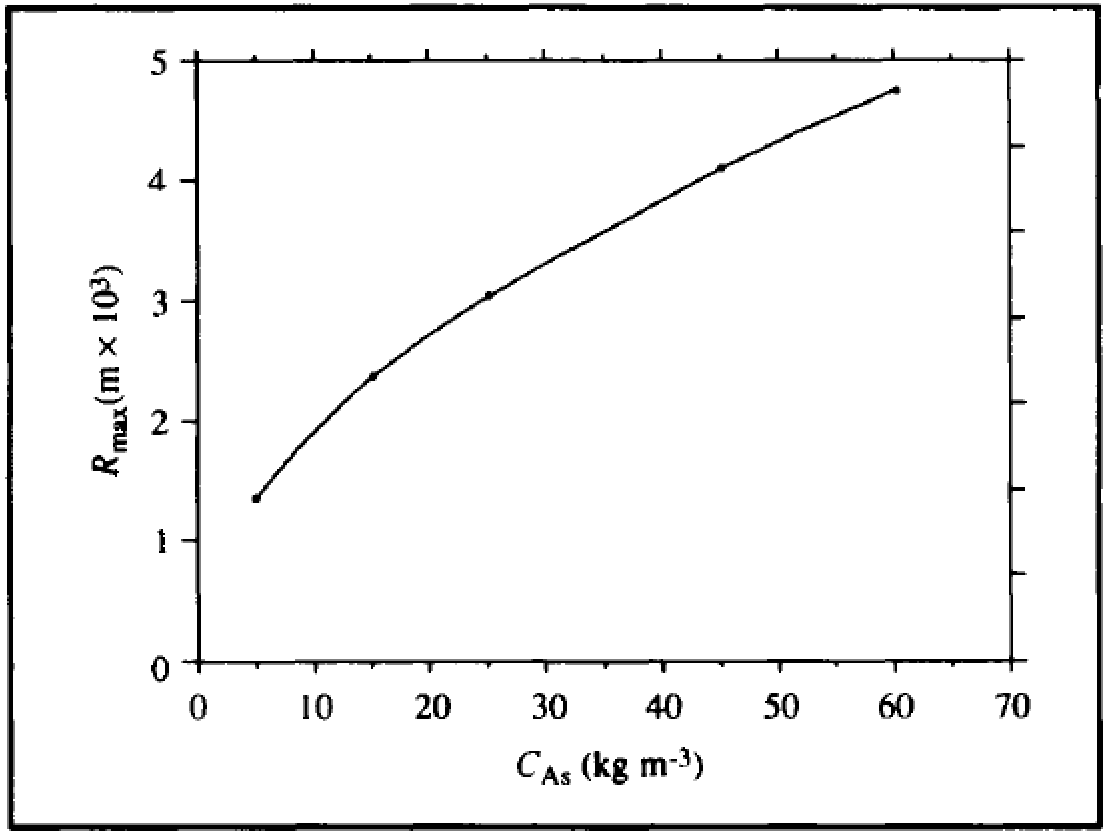
(a) At $y_C = 0.15$, $\mathscr{D}_{Ae} = 5.25 \times 10^{-10}\ \mathrm{m^2\ s^{-1}}$. Converting k_0 to units of kg, m and s:

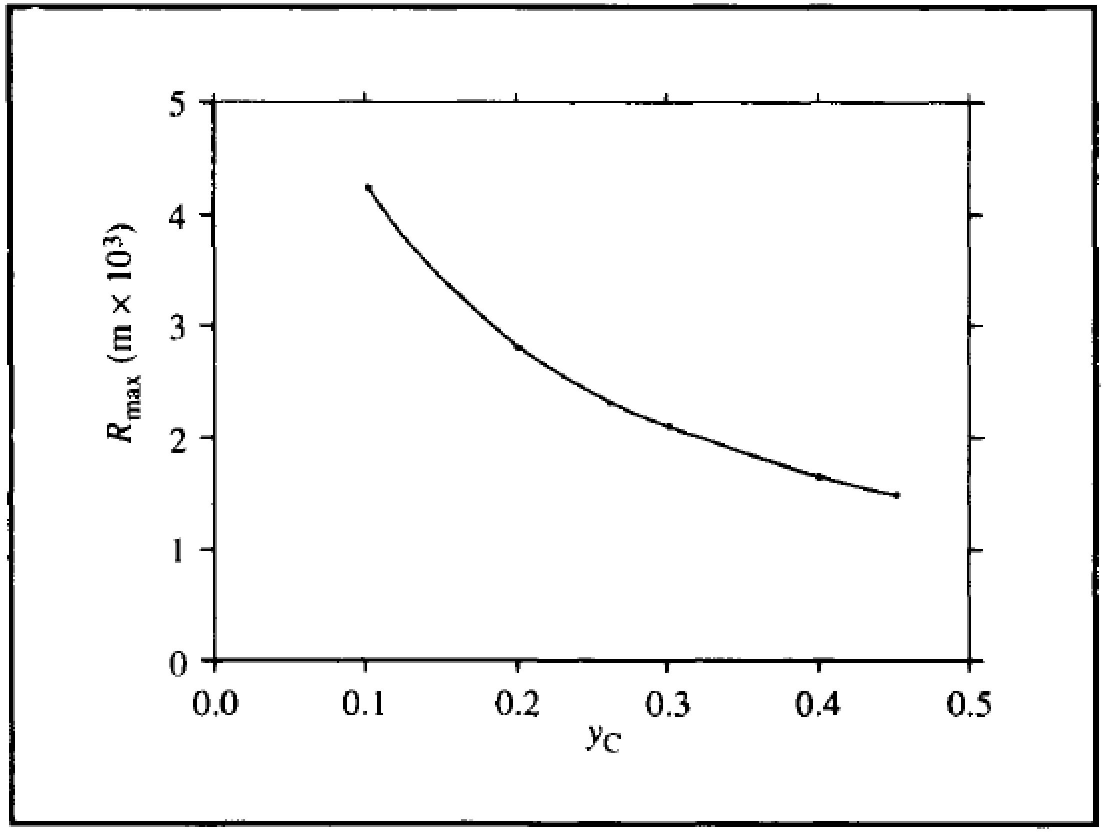
$$k_0 = 0.5\ \mathrm{g\ l^{-1}\ min^{-1}} \cdot \left| \frac{1\ \mathrm{kg}}{1000\ \mathrm{g}} \right| \cdot \left| \frac{1000\ \mathrm{l}}{1\ \mathrm{m^3}} \right| \cdot \left| \frac{1\ \mathrm{min}}{60\ \mathrm{s}} \right|$$

$$= 8.33 \times 10^{-3}\ \mathrm{kg\ m^{-3}\ s^{-1}}.$$

Assume C_{As} is equal to the bulk glucose concentration; C_{As} in $\mathrm{g\ l^{-1}}$ is the same as $\mathrm{kg\ m^{-3}}$. R_{max} is calculated from Eq

C_{As} ($\mathrm{kg\ m^{-3}}$)	R_{max} (m)
5	1.38×10^{-3}
15	2.38×10^{-3}
25	3.07×10^{-3}
45	4.13×10^{-3}
60	4.76×10^{-3}


R_{max} (m × 10^3)
C_{As} (kg m^{-3})
0
1
2
3
4
5
0
10
20
30
40
50
60
70


R_{max} (m × 10^3)
y_C
0
1
2
3
4
5
0.0
0.1
0.2
0.3
0.4
0.5

(b) $C_{As} = 30$ kg m^{-3}. As y_C varies, values of $\mathscr{D}_{Ae}$ and k_0 are affected. Changes in $\mathscr{D}_{Ae}$ can be calculated from the equation provided. We assume k_0 is directly proportional to cell density as described in Eq. (11.25), i.e. there is no steric hindrance or interaction between cells as y_C increases. Results as a function of y_C are listed below.

y_C	$\mathscr{D}_{Ae}$ (m^2 s^{-1})	k_0 (kg m^{-3} s^{-1})	R_{max} (m)
0.1	5.61×10^{-10}	5.55×10^{-3}	4.27×10^{-3}
0.2	4.90×10^{-10}	1.11×10^{-2}	2.82×10^{-3}
0.3	4.18×10^{-10}	1.67×10^{-2}	2.12×10^{-3}
0.4	3.46×10^{-10}	2.22×10^{-2}	1.67×10^{-3}
0.45	3.10×10^{-10}	2.50×10^{-2}	1.50×10^{-3}

The results are plotted in Figure 12E2.2. As y_C increases, $\mathscr{D}_{Ae}$ declines and k_0 increases. Lower $\mathscr{D}_{Ae}$ reduces the rate of diffusion into the particles; higher k_0 increases the demand for substrate. Therefore, increasing the cell density exacerbates mass-transfer restrictions. To ensure adequate supply of substrate under these conditions, the particle size must be reduced.