Bioreactor Equations

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December 15, 2021

1 Variables

Density: ρ
Velocity: $\boldsymbol{u}$
Time: t
Pressure: p
Gravitational acceleration: $\boldsymbol{g}$
Dynamic viscosity: μ
Oxygen volume concentration: C
Diffusion Coefficient: D
Nondimensional quantities are represented with an asterisk, *.

2 Dimensional Equations

2.1 PDEs

Navier-Stokes:

$$\rho\frac{\delta \boldsymbol{u}}{\delta t} + \rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\nabla p + \rho\boldsymbol{g} + \mu\nabla^2\boldsymbol{u} \tag{1}$$

Continuity:

$$\nabla\cdot\boldsymbol{u} = 0 \tag{2}$$

Advection-Diffusion:

$$\frac{\delta C}{\delta t} = D\nabla^2 C - \nabla\cdot(\boldsymbol{u}C) \tag{3}$$

2.2 Boundary Conditions

Dirichlet BCs for velocity (components of velocity correspond to “normal” and “tangential” directions):

$$\begin{aligned} \boldsymbol{u}(x, y_{top}, t) &= (0,0)\ m/s \\ \boldsymbol{u}(x_{top}, y, t) &= (0,0)\ m/s \\ \boldsymbol{u}(x, y_{bottom}, t) &= (0,0)\ m/s \\ \boldsymbol{u}(x_{bottom}, y, t) &= (0,0)\ m/s \end{aligned} \tag{4}$$

Boundary condition for tracer:

$$\frac{\delta C}{\delta \boldsymbol{n}}(x_{edge}, y_{edge}, t) = 0\ mol/m^3 \tag{5}$$

Where $\boldsymbol{n}$ is a vector perpendicular to the edge of the ellipse. In other words, the tracer boundary condition is non-source, Neumann in the direction perpendicular to the ellipse and free-slip in the tangential direction. The only exception to this is where $||\boldsymbol{u}|| > 0$ and $C > 0$ near the boundaries. In these conditions, Basilisk’s solvers will tend to introduce small erroneous source terms.

2.3 Initial Conditions

Velocities are initially 0.

$$\boldsymbol{u}(x, y, 0) = (0,0) \tag{6}$$

3 Scaling Parameters

Characteristic Length: L
Characteristic Speed: U
Gravitational Acceleration: g
Reference Pressure: p_0

4 Nondimensional Variables

Position: $\boldsymbol{x^*} = \frac{\boldsymbol{x}}{L}$
Velocity: $\boldsymbol{u^*} = \frac{\boldsymbol{u}}{U}$
Time: $t^* = \frac{t}{L/U}$
Pressure: $p^* = \frac{p}{\rho U^2}$
Concentration: $C^* = \frac{C}{C_0}$

5 Nondimensionalization

5.1 Nondimensionalizing the PDEs

Navier-Stokes (taking each term separately):

1.
$$\rho \frac{\delta \boldsymbol{u}}{\delta t} = \rho \frac{\delta(U\boldsymbol{u^*})}{\delta(\frac{L}{U}t^*)} = \frac{\rho U^2}{L}\frac{\delta u^*}{\delta t^*} \tag{7}$$

2.
$$\begin{aligned} \rho(\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} = \rho u_x \frac{\delta \boldsymbol{u}}{\delta x} + \rho u_y \frac{\delta \boldsymbol{u}}{\delta y} &= \rho(U u_x^*)\frac{\delta(U\boldsymbol{u^*})}{\delta(L\boldsymbol{x})} + \rho(U u_y^*)\frac{\delta(U\boldsymbol{u^*})}{\delta(L\boldsymbol{x^*})} \\ &= \frac{\rho U^2}{L}(u_x^*\frac{\delta \boldsymbol{u^*}}{\delta x^*} + u_y^*\frac{\delta \boldsymbol{u^*}}{\delta y^*}) \\ &= \frac{\rho U^2}{L}(\boldsymbol{u^*} \cdot \boldsymbol{\nabla^*})\boldsymbol{u^*} \end{aligned} \tag{8}$$

3.
$$-\nabla p = -\frac{\rho U^2}{L}\nabla^* p^* \tag{9}$$

4.
$$\rho \boldsymbol{g} = \rho g \hat{\mathbf{g}} \tag{10}$$

5.
$$\begin{aligned} \mu \nabla^2 \boldsymbol{u} = \mu(\frac{\delta^2 \boldsymbol{u}}{\delta x^2} + \frac{\delta^2 \boldsymbol{u}}{\delta y^2}) &= \mu(\frac{\delta^2(U\boldsymbol{u^*})}{\delta(Lx^*)^2} + \frac{\delta^2(U\boldsymbol{u^*})}{\delta(Ly^*)^2}) \\ &= \frac{\mu U}{L^2}(\frac{\delta^2 \boldsymbol{u^*}}{\delta x^{*2}} + \frac{\delta^2 \boldsymbol{u^*}}{\delta x^{*2}}) \\ &= \frac{\mu U}{L^2}\boldsymbol{\nabla^{*2} u^*} \end{aligned} \tag{11}$$

Adding up the terms and simplifying gives the following nondimensional Navier-Stokes equation:

$$\frac{\delta \boldsymbol{u^*}}{\delta t^*} + (\boldsymbol{u^*} \cdot \nabla^*)\boldsymbol{u^*} = -\nabla^* p^* + \frac{1}{Fr^2}\hat{\mathbf{g}} + \frac{1}{Re}\nabla^{*2}\boldsymbol{u^*} \tag{12}$$

5.2 Nondimensionalizing Continuity

$$\begin{aligned}\nabla \cdot \boldsymbol{u} = \frac{\delta u_x}{\delta x} + \frac{\delta u_y}{\delta y} &= \frac{\delta(U u_x^*)}{\delta(x^* L)} + \frac{\delta(U u_y^*)}{\delta(y^* L)} \\ &= \frac{U}{L}(\frac{\delta u_x^*}{\delta x^*} + \frac{\delta u_y^*}{\delta y^*}) \\ &= \frac{U}{L}(\boldsymbol{\nabla^*} \cdot \boldsymbol{u^*})\end{aligned} \tag{13}$$

And $\nabla \cdot \boldsymbol{u} = 0$, so

$$\boldsymbol{\nabla^*} \cdot \boldsymbol{u^*} = 0 \tag{14}$$

5.3 Nondimensionalizing Advection-Diffusion

$$\begin{aligned}\frac{\delta C}{\delta t} &= D\nabla^2 C - \nabla \cdot (\boldsymbol{u}C) = D(\frac{\delta^2 C}{\delta x^2} + \frac{\delta^2 C}{\delta y^2}) - u_x \frac{\delta C}{\delta x} - u_y \frac{\delta C}{\delta y} \\ &= D(\frac{\delta^2 C}{\delta(x^* L)^2} + \frac{\delta^2 C}{\delta(y^* L)^2}) - (u_x^* L)\frac{\delta C}{\delta(x^* L} - (u_y^* L)\frac{\delta C}{\delta(y^* L)} \\ &= \frac{D}{L^2}(\frac{\delta^2 C}{\delta x^{*2}} + \frac{\delta^2 C}{\delta y^{*2}}) - u_x^* \frac{\delta C}{\delta x^*} - u_y^* \frac{\delta C}{\delta y^*}\end{aligned} \tag{15}$$

Also,

$$\frac{\delta C}{\delta t} = \frac{\delta C}{\delta(t^* \frac{L}{U}})) \tag{16}$$

Setting these equal gives

$$\frac{\delta C}{\delta t^*} = \frac{D}{UL}\nabla^{*2} C - \nabla^* \cdot (\boldsymbol{u^*}C) \tag{17}$$

Plugging in $C^* = \frac{C}{C_0}$ gives

$$\frac{\delta(C^* C_0)}{\delta t^*} = \frac{D}{UL}\nabla^{*2}(C^* C_0) - \nabla^* \cdot (\boldsymbol{u^*}C^* C_0) \tag{18}$$

The C_0 cancels, giving

$$\frac{\delta C^*}{\delta t^*} = \frac{D}{UL}\nabla^{*2} C^* - \nabla^* \cdot (\boldsymbol{u^*}C^*) \tag{19}$$

With the Peclet number defined $Pe = \frac{UL}{D}$, I get

$$\frac{\delta C^*}{\delta t^*} = \frac{1}{Pe}\nabla^{*2} C^* - \nabla^* \cdot (\boldsymbol{u^*}C^*) \tag{20}$$

5.4 Nondimensionalizing Boundary Conditions

Taking the dimensional boundary conditions and substituting in $\boldsymbol{u} = U\boldsymbol{u^*}$ and $\boldsymbol{x} = \boldsymbol{L}\boldsymbol{x^*}$ gives:

$$\begin{aligned}\boldsymbol{u^*}(x^*, y^*_{top}, t^*) &= (0,0) \\ \boldsymbol{u^*}(x^*_{top}, y^*, t^*) &= (0,0) \\ \boldsymbol{u}(x^*, y^*_{bottom}, t^*) &= (0,0) \\ \boldsymbol{u}(x^*_{bottom}, y^*, t^*) &= (0,0)\end{aligned} \tag{21}$$

Tracer Boundary Condition:

$$\frac{\delta C^*}{\boldsymbol{n^*}}(x^*_{edge}, y^*_{edge}, t^*) = 0 \tag{22}$$

5.5 Nondimensionalizing Initial Condition

Similar reasoning gives $\boldsymbol{u^*}(x^*, y^*) = (0,0)$ for $t = 0$.
Not sure how to deal with the tracer initial condition...?

6 Listing all the Parameters

6.1 Dimensional Parameters

Since there are two fluids in the reactor, there are two values for ρ, μ, and Pe.
Water density: $\rho_{water} = 1000.0 \ \frac{kg}{m^2}$
Air density: $\rho_{air} = 1.225 \ \frac{kg}{m^2}$
Water dynamic viscosity: $\mu_{water} = 0.001 \ Pa \cdot s$ at 20 C
Air dynamic viscosity: $\mu_{air} = 1.81 \times 10^-4 \ Pa \cdot s$ (multiplied by 10)
Water-air surface tension: $\sigma = 0.0728 \ \frac{N}{m}$
Semimajor axis length: $a = 3.0$ cm $= 0.03$ m
Semiminor axis length: $b = 1.0$ cm $= 0.01$ m
Fill height: 0.3 (filled halfway)
Max. angle of rotation: $\Theta = 7° = 0.12217$ Rad
Rocking Period: $T = 1$ s (let's say for now - this turns out to be almost exactly what my rocking period has been in initial simulations, and roughly lines up with videos sent from Dan as well as the setup in Zhan et al.)
Reference Length: $L = 0.01$ m
Reference Velocity: $U = \frac{b\Theta}{T} = \frac{0.01*0.12217}{1.0} = 0.0012217$ m/s
Not technically one of the dimensional parameters, but useful to include: Reference time scale: $\frac{L}{U} = 8.1851$ s. This means that in nondimensional terms, the period of oscillation should be set to $\frac{1}{L/U} = 1/8.1851 = 0.12217$. This differs DRASTICALLY from my original setup, which had the period of oscillation set to 80 nondimensional seconds.
Gravitational acceleration (magnitude): $g = 9.8$ m/s
O2 diffusion coefficient in air (? double check): $D_{air} = 1.98 \times 10^-5 \ \frac{m^2}{s}$
O2 diffusion coefficient in water (? double check): $D_{water} = 1.90 \times 10^-9 \ \frac{m^2}{s}$
(should check at some point that these coefficients are for the correct temperature) *Diffusion time scales (not actually part of the needed parameters):* $\tau_{water} = \frac{L^2}{D_{water}} = 52,631.58 \ s$, $\tau_{air} = \frac{L^2}{D_{air}} = 5.05 \ s$

6.2 Nondimensional Parameters

Froude Number: $Fr = \frac{U}{\sqrt{gb}} = \frac{0.0012217}{\sqrt{9.8 \times 0.01}} = 0.003903$
Reynolds Number: $Re = \frac{\rho_{water} UL}{\mu_{water}} = \frac{1,000 \cdot 0.0012217 \cdot 0.01}{0.001} = 12.2173$
Weber Number: $We = \frac{\rho_{water} U^2 L}{\sigma} = \frac{1,000 \cdot 0.0012217^2 \cdot 0.01}{0.0728} = 0.000205$
Density Ratio: $\frac{\rho_{air}}{\rho_{water}} = 0.001225$
Viscosity Ratio: $\frac{\mu_{air}}{\mu_{water}} = 0.181$
Aspect Ratio of Container: 3.0
Fill portion: 0.5 (filled halfway)
Water Peclet Number: $Pe_{water} = \frac{UL}{D_{water}} = 6,430$
Air Peclet Number: $Pe_{air} = \frac{UL}{D_{air}} = 0.617$

7 Alternative Parameters

To get nicer nondimensional parameters for the purposes of computation, I will set the Froude number to 1.0 and define the reference velocity as $U = Fr \cdot \sqrt{gL}$. This formulation causes U to be significantly larger in the simulation than in my physical setup. In other words, for a given rocking period, the computational nondimensionalization will treat the rocking motion as being more violent than it actually is, by a factor equal to the discrepancy in reference velocities. However, the nondimensional rocking period is equal to the rocking period divided by the reference time scale, and the difference between the reference velocities causes a corresponding difference in the reference time scales, which allows the nondimensional rocking period to be adjusted appropriately.
The following table compares parameters between the physical and computational setups. Parameters that are different between the two setups are in red, and parameters that are useful to know but not actually part of the nondimensionalization are highlighted. There is a small separation between the

portion of the table handling dimensional parameters and the portion with nondimensional parameters.

Parameter	**Physical Setup**	**Computational Setup**
Water density ρ_{water} (kg/m^3)	1000.0	1000.0
Air density ρ_{air} (kg/m^3)	1.225	1.225
Water dynamic viscosity μ_{water} $(Pa \cdot s)$	0.001	0.001
Air dynamic viscosity μ_{air} $(Pa \cdot s)$	1.81×10^{-4}	1.81×10^{-4}
Water-air surface tension σ (N/m)	0.0728	0.0728
Semimajor axis length a (m)	0.03	0.03
Semiminor axis length b (m)	0.01	0.01
Fill height (m)	0.3	0.3
Max. angle of rotation Θ (radians)	0.12217	0.12217
Rocking period T (s)	**1.0**	**1.0**
Reference Length L (m)	0.01	0.01
Reference Velocity U (m/s)	$\frac{b\Theta}{T} = 0.0012217$	$Fr \cdot \sqrt{(}gL) = 1.0 \cdot \sqrt{(}9.8 \cdot 0.01) = 0.3130$
Reference time scale $T_{ref} = L/U$ (s)	8.1853	$= 0.03194$
Gravitational acceleration g (m/s^2)	9.8	9.8
O2 diffusion coefficient in air D_{air} (m^2/s)	1.98×10^{-5}	1.98×10^{-5}
O2 diffusion coefficient in water D_{water} (m^2/s)	1.90×10^{-9}	1.90×10^{-9}
Diffusion time scale in water $\tau_{water} = L^2/D_{water}$ (s)	52,631.58	52,631.58
Diffusion time scale in air $\tau_{air} = L^2/D_{air}$ (s)	5.05	5.05
Nondimensional Rocking Period $T^* = T/T_{ref}$	0.12217	31.305
Froude Number $Fr = U/\sqrt{gb}$	**0.00390**	**1.0**
Reynolds Number $Re = (\rho_{water}UL)/\mu_{water}$	**12.2173**	**3,130.4952**
Weber Number $We = (\rho_{water}U^2L)/\sigma$	**0.000205**	**13.4615**
Density Ratio ρ_{air}/ρ_{water}	0.001225	0.001225

Viscosity Ratio μ_{air}/μ_{water}	0.181	0.181
Aspect Ratio	3.0	3.0
Fill portion	0.5	0.5
Water Peclet Number $Pe_{water} = (UL)/D_{water}$	**6,430**	**1,647,629.036**
Air Peclet Number $Pe_{air} = (UL)/D_{air}$	**0.617**	**158.1058**

As can be seen in the table, the reference velocity in the computational setup is $\frac{0.3130}{0.0012217} = 256.20$ times larger than the reference velocity in the physical setup.

8 Full-sized reactor

Same table as above, but with a full-sized reactor with a semiminor axis of 0.1 m instead of 0.01 m, and a semimajor axis of 0.3 m:

Parameter	**Physical Setup**	**Computational Setup**
Water density ρ_{water} (kg/m^3)	1000.0	1000.0
Air density ρ_{air} (kg/m^3)	1.225	1.225
Water dynamic viscosity μ_{water} $(Pa \cdot s)$	0.001	0.001
Air dynamic viscosity μ_{air} $(Pa \cdot s)$	1.81×10^{-4}	1.81×10^{-4}
Water-air surface tension σ (N/m)	0.0728	0.0728
Semimajor axis length a (m)	0.3	0.3
Semiminor axis length b (m)	0.1	0.1
Fill height (m)	0.3	0.3
Max. angle of rotation Θ (radians)	0.12217	0.12217
Rocking period T (s)	**1.0**	**1.0**
Reference Length L (m)	0.1	0.1
Reference Velocity U (m/s)	$\frac{b\Theta}{T} = 0.012217$	$Fr \cdot \sqrt(gL) = 1.0 \cdot \sqrt(9.8 \cdot 0.01) = 0.9899$
Reference time scale $T_{ref} = L/U$ (s)	8.1853	0.101
Gravitational acceleration g (m^2)	9.8	9.8
O2 diffusion coefficient in air D_{air} (m/s^2)	1.98×10^{-5}	1.98×10^{-5}
O2 diffusion coefficient in water D_{water} (m/s^2)	1.90×10^{-9}	1.90×10^{-9}
Diffusion time scale in water $\tau_{water} = L^2/D_{water}$ (s)	5,263,158.0	5,263,158.0

Diffusion time scale in air $\tau_{air} = L^2/D_{air}$ (s)	505	505
Nondimensional Rocking Period $T^* = T/T_{ref}$	0.12217	9.899
Froude Number $Fr = U/\sqrt{gb}$	**0.01234**	**1.0**
Reynolds Number $Re = (\rho_{water}UL)/\mu_{water}$	**1,221.7**	**98,994.94936**
Weber Number $We = (\rho_{water}U^2L)/\sigma$	**0.205**	**1,346.15**
Density Ratio ρ_{air}/ρ_{water}	0.001225	0.001225
Viscosity Ratio μ_{air}/μ_{water}	0.181	0.181
Aspect Ratio	3.0	3.0
Fill portion	0.5	0.5
Water Peclet Number $Pe_{water} = (UL)/D_{water}$	**643,000**	**52,102,604.92**
Air Peclet Number $Pe_{air} = (UL)/D_{air}$	**61.7**	**4,999.74**