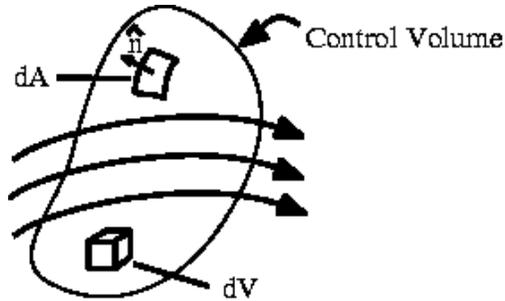

Differential Balance Equations (DBE)

Differential Balance Equations

Differential balances, although more complex to solve, can yield a tremendous wealth of information about ChE processes. General balance equations for each of the modes of transport can easily be derived either directly from shell balances or via control volume analysis. Understanding the origin and meaning of the terms that make up these balance equations lies at the heart of posing and solving complex transport problems.

- Describe the physical meaning of each of the terms within a general thermal energy balance
 - # Simplify the general thermal energy balance equation (identifying assumptions)
 - # Identify reasonable boundary conditions in a conduction problem (explain when each is most useful)
 - Describe the physical meaning of each of the terms within a differential mass balance equation
 - # Simplify the mass balance equation (identifying assumptions)
 - # Identify reasonable boundary conditions in a mass transport problem (explain when each is most useful)
 - Describe the physical meaning of each of the terms within the momentum balance
 - # Explain the physical meaning of the terms in the differential Continuity and Navier-Stokes Equations
 - # Simplify both the differential Continuity and Navier-Stokes Equations
 - # Identify proper boundary conditions for use with the Navier-Stokes equations
-

DBE: General Thermal Energy (Heat) Balance



For our balance, we will choose an **arbitrary** fixed (in space) control volume. Thus, it is an *open* system (i.e., one through which mass may flow). Accounting for *heat* within that control volume (and exchanged with its surroundings), we get:

rate of accumulation of **heat** in CV = $\text{net rate of heat transport into CV (by flow)}$ + $\text{net rate of heat transferred to material in CV}$ + $\text{net rate of heat "generation" in CV}$

It is useful to discuss why we must now include a "generation" term. This term originates from the fact that heat can be "made" from other forms of energy (friction, chemical reactions, electrical resistance, etc.). A very important point therefore is that *heat is not conserved!*

In writing this mathematically, we use cT to represent the thermal energy per unit mass, where c is the *heat capacity* of the material. We then get:

$$\frac{\partial}{\partial t} \iiint_{CV} \rho c T dV = - \iint_{CS} \rho c T (\mathbf{v} \cdot \mathbf{n}) dA - \iint_{CS} \left(\frac{q}{A} \cdot \mathbf{n} \right) dA + \iiint_{CV} \dot{q} dV$$

NOTATION:

- - \mathbf{Q} is the *flux* of heat to or from the material within the CV (the sign is chosen such that heat flowing *into* the material is positive).
- \dot{q} is the volumetric rate of thermal energy generation.

Now for a little bit of math wizardry...

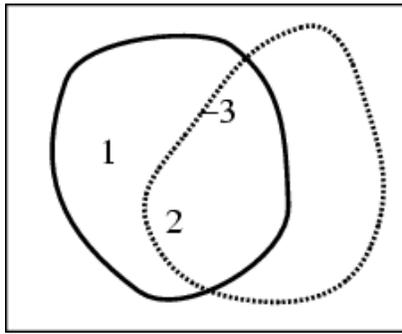
There is a theorem attributed to Gauss which states that a surface integral of a quantity can be written as a volume integral of the derivative of that quantity. Using this idea (and rearranging a little), we can write the heat balance instead as:

$$\iiint_{CV} \left\{ \frac{\partial}{\partial t} (\rho c T) + \nabla \cdot (\rho c T \mathbf{v}) + \nabla \cdot \left(\frac{q}{A} \right) - \dot{q} \right\} dV = 0$$

As we chose an **arbitrary** control volume, in order for this integral to be equal to zero for *any* choice of CV, the integrand must be zero. So, we now have a differential heat balance equation:

$$\frac{\partial}{\partial t} (\rho c T) = - \nabla \cdot (\rho c T \mathbf{v}) - \nabla \cdot \left(\frac{q}{A} \right) + \dot{q}$$

The best way to prove this "zero" thing to you is by contradiction:



Simplifying the GTEB

At the simplest level there are four assumptions that we can make that effect the terms within the General Thermal Energy Balance (GTEB) Equation:

- **Steady State** -- this assumption clearly affects the first term on the left-hand side ($d/dt = 0$); if it is *not* true we should try the Biot number to see if "lumped" is a more appropriate equation to solve
- **No Flow** -- this assumption is valid for solids or for truly stagnant fluids, it makes the first term on the right-hand side of the GTEB become zero
- **No Generation** -- this assumption requires that we have no chemical reactions, electrical current, frictional or mechanical work, etc. that might be turned into thermal energy, if true it makes the last term on the right-hand side become zero
- **Constant Properties** -- this is the trickiest assumption because it requires that we envision having only a small-to-moderate overall temperature *span* within our material of interest (particularly difficult to assess when we have generation), if it holds true we pull the density, heat capacity, and conductivity (in the function Q) out of all derivatives

OUTCOME:

Simplify the general thermal energy balance equation (identifying assumptions)

NOTE:

In order to "set up the equation", one needs to not only write and simplify the appropriate form of this differential equation, but also include the relevant boundary conditions!

DBE: Thermal Boundary Conditions

1ST KIND:

We can specify the temperature at the boundaries (on either side of a slab for example $T=T_1$ at x_1 and $T=T_2$ at x_2). This is known as the Dirichlet condition or boundary condition of the first kind.

NOTE:

*It is critical that we realize that we can only use this condition if we actually know a **value** for the temperature (for example, $T_1=50C$)*

2ND KIND:

We can specify a constant *flux* at the boundary (for example, $-k\frac{dT}{dx} = C$ at some position x_1). This is known as a Neumann or second kind condition.

NOTE:

*Again, we must know the **value** of the flux, C . The special case where this is equal to zero is the insulated or adiabatic boundary condition.*

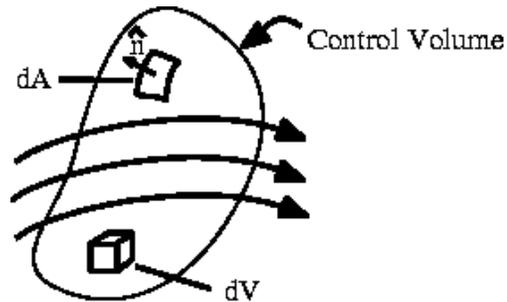
3RD KIND:

Finally, we can combine the two, and specify that the flux is somehow related to the temperature (for example, $-k\frac{\partial T}{\partial y} = h(T-T_\infty)$). This is called the Robin or third type. (The special case shown here is the convection condition, but it could also be radiation, etc.).

OUTCOME:

Identify reasonable boundary conditions in a heat transfer problem (explain when each is most useful)

DBE: General Material Balance



For our balance, we will choose an **arbitrary** fixed (in space) control volume. Thus, it is an *open* system (i.e., one through which mass may flow). Accounting for mass within that volume (and transferred with surroundings) we get:

$$\begin{aligned} \text{rate of accumulation} &= \text{net rate of mass} &+ \text{net rate of mass} \\ \text{of mass in CV} &= \text{transport into CV} &+ \text{"generation" in CV} \end{aligned}$$

Here the "generation" term arises due to our balance being focused on a *specific* type of material, so reactions can generate/consume it.

In writing this mathematically, we use c_i for a balance on a molar basis and ρ for a balance based on mass. We then get:

$$\frac{\partial}{\partial t} \iiint_{CV} \rho_i dV = - \iint_{CS} \rho_i (v_i \cdot n) dA + \iiint_{CV} \dot{r}_i dV$$

If we use the definition of the mass flux vector (of component i), $n_i = \rho_i v_i$, we can re-write this equation as:

$$\frac{\partial}{\partial t} \iiint_{CV} \rho_i dV = - \iint_{CS} (n_i \cdot n) dA + \iiint_{CV} \dot{r}_i dV$$

Now using the same bit of math wizardry that we used before (i.e., the Gauss divergence theorem) ...

$$\iiint_{CV} \left[\frac{\partial \rho_i}{\partial t} + \nabla \cdot n_i - \dot{r}_i \right] dV = 0$$

Again, since we chose an **arbitrary** control volume, the integrand must be zero. So, we now have a differential material balance equation:

$$\frac{\partial \rho_i}{\partial t} = -\nabla \cdot n_i + \dot{r}_i$$

We could write the same equation in terms of molar concentrations by dividing by the molecular weight of the material:

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot N_i + \dot{R}_i$$

Simplifying the GMB

Unlike the GTEB, the General Mass Balance (GMB) equation has only three assumptions/conditions that we can make that to simplify our problems:

- **Steady State** -- this assumption clearly affects the first term on the left-hand side ($d/dt = 0$); if it is *not* true we should try the Biot number to see if "lumped" is a more appropriate equation to solve
- **No Reaction** -- this assumption requires that we have no chemical reactions, if true it makes the last term on the right-hand side become zero

- **Driven or Diffusion-induced Flow** -- this is not exactly an "assumption", but is an ascertainment that must be made when solving problems. Using the definition of the total material flux, we obtain the average velocity either through "flux balancing" (see the section on constitutive laws) or directly from knowledge of the velocity field

OUTCOME:

Simplify the general material energy balance equation (identifying assumptions)

DBE: Material Boundary Conditions

1ST KIND:

A very common boundary condition for mass transfer is to know the concentration at the boundaries. This could happen for several physically realistic reasons: you measure the concentration, the boundary is between phases and you have equilibrium data that tells you the concentration (i.e., the boundary (interface) is at the saturation concentration), you have a rapid (infinitely fast) reaction occurring at the boundary so that the concentration at there is zero.

NOTE:

*As with heat transfer, it is critical that we realize that we can only use this condition if we actually know a **value** for the concentration*

2ND KIND:

We can specify a constant *flux* at the boundary. This is useful as the symmetry condition (at the center of a sphere or cylinder) where the flux would be zero, if we know that one boundary is impenetrable so that the flux is zero, if we know what the value of the rate of reaction is (since we could set the flux at the boundary equal to this value), or if we simply measure the flux/flow of mass.

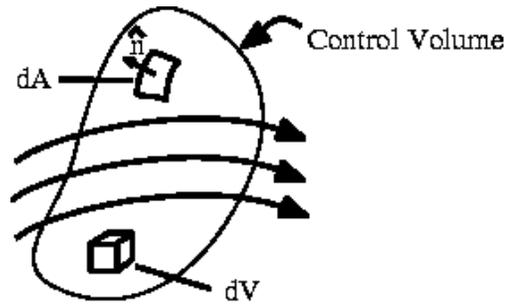
3RD KIND:

Again, we can combine the two, and specify that the flux is somehow related to the concentration. This would happen at an interphase boundary where we might know that diffusion is equal to convection.

OUTCOME:

Identify reasonable boundary conditions in a mass transfer problem (explain when each is most useful)

DBE: Navier-Stokes Equations (Momentum Balance Equations)



For our balance, we will choose an **arbitrary** fixed (in space) control volume. Thus, it is an *open* system (i.e., one through which mass may flow). Accounting for momentum within that volume (and transferred with surroundings) we get:

rate of accumulation of momentum in CV = *net* rate of momentum transport *into* CV + sum of the forces acting on the CV

Writing this mathematically, we get:

$$\frac{\partial}{\partial t} \iiint_{CV} \rho \vec{v} dV = - \iint_{CS} \rho \vec{v} (\vec{v} \cdot \vec{n}) dA + \sum \vec{F}$$

where the sum of the forces includes two classes of force:

$$\sum \vec{F} = \sum \vec{F}_{body} + \sum \vec{F}_{surface}$$

The body forces could include magnetic and/or electrical forces, but generally only include gravitational:

$$\sum \vec{F}_{body} = \iiint_{CV} \rho \vec{g} dV$$

The surface forces include shear and normal stresses. For a Newtonian fluid, the only normal stresses we will consider are pressure stresses so we get:

$$\sum \vec{F}_{surface} = - \iint_{CS} P \cdot \vec{n} dA + \iint_{CS} \vec{\tau} dA$$

NOTE:

The pressure must be dotted into the normal vector because the pressure has no direction; however, by convention we do give the pressure a sign convention so that it is positive when compressive. This is why we include the negative sign here (compression is opposite the normal vector).

Combining these expressions gives us:

$$\frac{\partial}{\partial t} \iiint_{CV} \rho \vec{v} dV = - \iint_{CS} \rho \vec{v} (\vec{v} \cdot \vec{n}) dA + \iiint_{CV} \rho \vec{g} dV - \iint_{CS} P \cdot \vec{n} dA + \iint_{CS} \vec{\tau} dA$$

Now using the same bit of math wizardry that we used before (i.e., the Gauss divergence theorem) and rearranging things

$$\iiint_{CV} \left[\frac{\partial(\rho\vec{v})}{\partial t} + \nabla \cdot (\rho\vec{v}\vec{v}) - \rho\vec{g} + \nabla P - \nabla \cdot \vec{\tau} \right] dV = 0$$

With our **arbitrary** control volume, the integrand must be zero. So, we now have a differential momentum balance equation:

$$\frac{\partial(\rho\vec{v})}{\partial t} + \nabla \cdot (\rho\vec{v}\vec{v}) = \rho\vec{g} - \nabla P + \nabla \cdot \vec{\tau}$$

The left hand side of this equation is often called the substantial or lagrangian time derivative as this is the time derivative that "follows" the fluid (because of the inclusion of the advective second part):

$$\frac{\partial(\rho\vec{v})}{\partial t} + \nabla \cdot (\rho\vec{v}\vec{v})$$

If we are interested in only incompressible, Newtonian fluids we get the final form of the Navier-Stokes equations as:

$$\rho \frac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \nabla \vec{v} = \rho \vec{g} - \nabla P + \mu \nabla^2 \vec{v}$$

Simplifying the Navier-Stokes Equations

The first thing to note about the N-S equations, is that there are three of them!

$$\begin{aligned} \rho \frac{\partial v_x}{\partial t} + \rho(v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z}) &= \rho g_x - \frac{\partial P}{\partial x} + \mu(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}) \\ \rho \frac{\partial v_y}{\partial t} + \rho(v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z}) &= \rho g_y - \frac{\partial P}{\partial y} + \mu(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2}) \\ \rho \frac{\partial v_z}{\partial t} + \rho(v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z}) &= \rho g_z - \frac{\partial P}{\partial z} + \mu(\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2}) \end{aligned}$$

Unlike the previous equations, there are only two assumptions/conditions that we can make here:

- **Steady State** -- this assumption clearly affects the first term on the left-hand side ($d/dt = 0$)
- **Laminar Flow** -- this assumption allows us to rationalize which velocities (v_i) and which **derivatives** of velocities ($d v_i / d x_j$) can be omitted from our equations

NOTE:

*The equation that we derived **required** that we also assume that we are dealing with an incompressible and Newtonian fluid.*

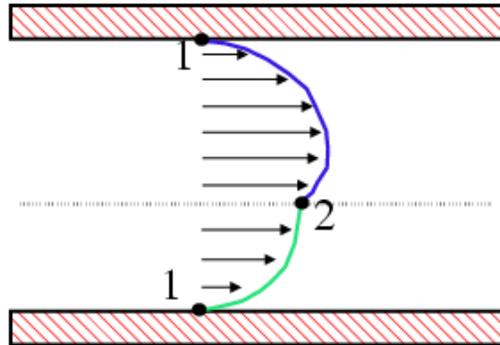
OUTCOME:

Simplify the general material energy balance equation (identifying assumptions)

DBE: Fluid Mechanics Boundary Conditions

1ST KIND:

The **most** common boundary condition for fluid mechanics is to know the concentration at the boundaries. This arises primarily as the *no slip condition*. The no slip condition means that the fluid velocity at the boundary is equal to the boundary's velocity. This holds true both for fluid-solid boundaries (which might be zero like at point(s) 1) as well as fluid-fluid boundaries. (where the two fluids have the same velocity, like at point 2).



2ND KIND:

We can specify a constant *flux* at the boundary when we know the value of the *stress* there (i.e., knowing the momentum flux). The most common place that this would arise would be as a continuity of stress condition at the boundary between two fluids. (At point 2 notice that the slopes of the velocity profiles have the same *sign*, but not necessarily the same value of the slope, because the viscosities may be different)

$$\mu_A \frac{\partial v_{xA}}{\partial y} = \mu_B \frac{\partial v_{xB}}{\partial y}$$

A special case of this is for the case of $\mu_A \gg \mu_B$ where we assume that $\frac{\partial v_{xA}}{\partial y} \approx 0$

3RD KIND:

Not common in fluid mechanics.

OUTCOME:

Identify reasonable boundary conditions in a fluid mechanics problems (explain when each is most useful)
