ChE 240: Fluid Flow and Heat Transfer
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I. INTRODUCTION

For most of you, this is your second course in the chemical engineering department. The first course, ChE 200: Fundamentals of Chemical Engineering, focussed on material and energy balances. This is an appropriate place to start a study of Chemical Engineering because:

Engineering is the study of solutions to (applied) balance equations.

What does this statement mean? It means that 90% of what engineers do (including chemical engineers) is to solve problems by (a) formulating balance equations which describe the problem and (b) solving the balance equations. At least, this is my perspective on the big picture of chemical engineering. (Balance equations have other names as well. They are also called conservation equations. In fluid dynamics, a mass balance is referred to as continuity equation. Whatever the name, balance equations are at the core of Chemical Engineering.)

This second course in the Chemical Engineering curriculum, ChE 240: Fluid Flow and Heat Transfer, is a continuation of the study of balance equations begun in ChE 200. In ChE 240, we apply balance equations to solve problems of fluid flow and heat transfer. When we look at fluid flow problems, most typically we are interested in material (mass or mole) balances, momentum balances, and mechanical energy balances. When we look at heat transfer problems, we frequently are interested in heat balances. Much of the time, the fluid flow and heat transfer problems are coupled (inextricably connected) and we have to solve a system of such balance equations simultaneously.

Why is it important to realize that Chemical Engineering (and specifically the content of ChE 240) is simply the solution of applied balance equations? This realization is important because, as we look at complex problems, there will be all kinds of details that pop up and may confuse us. We not be able to see the forest for the trees. So here, at the beginning, we see the forest is just a system of balance equations. When the forest becomes tangled and dense with all sorts of complicated terms, we may lose our bearings, but so long as we have a fundamental understanding of what a balance equation is, we can always re-orient ourselves and proceed to the solution of the problem.

In the syllabus, we have listed 24 specific objectives for this course but there are a few generalized objectives which summarize all of the more specific ones. These general objectives are to

- examine different types of balance equations, commonly encountered in chemical engineering problems dealing with fluid flow and heat transfer
- provide methodical solution strategies for solving these balance equations
- gain a familiarity and proficiency with the periphery calculations associated with solving balance equations, e.g. unit conversions.

- apply balance equations to chemical engineering systems.

II. BALANCE EQUATIONS

So here we are about to enter the forest of fluid flow and heat transfer. What are we going to use as our compass to guide us? My suggestion is the generalized balance equation:

KEY POINT: THE BALANCE EQUATION

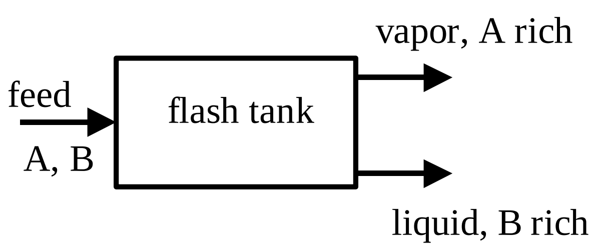
$$\text{accumulation} = \text{in} - \text{out} + \text{generation} - \text{consumption} \tag{1}$$

Believe it or not, you will never encounter a chemical engineering problem where this statement does not hold true. If Chemical Engineering is just about solving this equation, you may wonder why it takes four years to get a Bachelors of Science degree in Chemical Engineering. Of course, the reason is that there are infinite variations to this equation. You spend time at the University making yourself familiar with the most common applications of this equation.

Let's take a look at some examples of balance equations. Some of these may be familiar from ChE 200 and some may not. Nevertheless, in all cases, you ought to see the fundamental balance equation at work:

Mass balance: (a separation example from the chemical industry)

We want to separate a mixture of A and B in a flash tank, a unit which takes a single-phase vapor and separates it into two effluent streams, one vapor, one liquid. Let's say that component A in the feed is more volatile than component B so that the vapor produced contains more A than the feed stream did. (The vapor is A rich.) The liquid contains more B. The system runs continuously at "steady-state" so there is no accumulation.

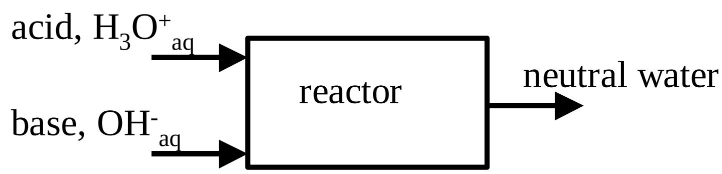


The **mass** balances for A and B are:

$$\begin{aligned}
\text{acc} &= \text{in} - \text{out} + \text{gen} - \text{con} \\
0 &= \text{A in feed} - (\text{A in vapor} + \text{A in liquid}) + 0 - 0 \\
0 &= \text{B in feed} - (\text{B in vapor} + \text{B in liquid}) + 0 - 0
\end{aligned} \tag{2}$$

There is no reaction so there is no generation or consumption. It is fairly to see from this example, familiar to you from ChE 200, how the generalized balance equation is used.

Mole balance: (an example from the chemical industry)
We want to neutralize an acid with a base in a reactor vessel, operating at steady state.

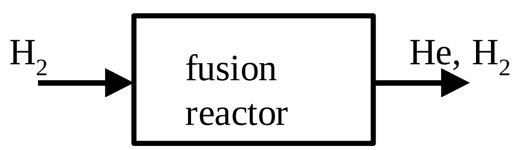


The **mole** balances for acid and base are:

$$\begin{array}{lllllll} acc = & in & - & out & + gen & - & con \\ 0 = & H_3O^+ \text{ in} & - & H_3O^+ \text{ out} & + \ 0 & - & H_3O^+ \text{ consumed by } OH^- \\ 0 = & OH^- \text{ in} & - & OH^- \text{ out} & + \ 0 & - & OH^- \text{ consumed by } H_3O \end{array} \quad (3)$$

Here, since we have reaction, we have hydronium and hydroxide ions consumed. Again, the application of the generalized balance equation should be obvious.

Atom balance: (a reaction example)
In a hypothetical fusion reactor, hydrogen combines to form helium and release energy. However, not all of the hydrogen fed into the reactor reacts; some leaves with the helium.



The **atom** balances for H and He are, respectively:

$$\begin{array}{lllllllll} acc = & in & - & out & + & gen & - & con \\ 0 = & 2H_2 \text{ in} & - & 2H_2 \text{ out} & + & 0 & - & 2H_2 \text{ consumed} \\ 0 = & 0 & - & \text{He out} & + & H_2 \text{ consumed} & - & 0 \end{array} \quad (4)$$

Since the balances are over elements there are 2's in front of each H_2, since they contain 2 atoms of H. Again, the application of the generalized balance equation should be obvious.

Polymer molecular weight balance: (from polymer engineering)
A polymer is a large molecule created by connecting together many small molecules, called monomers, (frequently of the same type). A polymer of size i is labeled as species P_i and contains i monomers. If we just dump the monomer in a reactor, we begin to form some

distribution of P_i, with i ranging from 1 (monomer) to perhaps several million. We then have many million mole balances, one for each value of i. Let's say our reactor is a batch reactor; a cauldron with no in and no out terms. A batch reactor is also not a steady-state system, so we have accumulation.

The generation term comes from reactions. For example, a polymer of size i=2, P_2, is formed by the reaction of P_1+P_1. A polymer of size 4, P_4, is formed by the reaction of P_2+P_2 or P_1+P_3. Therefore, the generation term of a P_4 polymer contains elements of the consumption terms for P_1, P_2, and P_3. Thus, in general, P_i can be made by any reaction of P_j and P_{i-j}, where j < i. The reaction rate constant for this combination of P_j and P_{i-j} is $k_{j,i-j}$.

The **polymer** balances for P_i, where i ranges from 1, 2, 3… to many million (i_{max}) are:

$$\begin{array}{ccccccc} \mathrm{acc} & = \mathrm{in} - \mathrm{out} + & \mathrm{gen} & - & \mathrm{con} \\ \dfrac{dP_i}{dt} & = 0 - \ \ 0 \ \ + & \sum\limits_{j<i}^{i_{max}}\left(k_{j,i-j}P_jP_{i-j}\right) & - & \sum\limits_{j>i}^{i_{max}}\left(k_{i,j-i}P_iP_{j-i}\right) \end{array} \quad (5)$$

or, for example, i = 4, with $i_{max} = 6$

$$\begin{array}{ccccccc} \mathrm{acc} & = \mathrm{in} - \mathrm{out} + & \mathrm{gen} & - & \mathrm{con} \\ \dfrac{dP_4}{dt} & = 0 - \ \ 0 \ \ + & \left(k_{1,3}P_1P_3 + k_{2,2}P_2P_2\right) & - & \left(k_{1,4}P_1P_4 + k_{2,4}P_2P_4\right) \end{array}$$

The generation term includes the reactions: $P_2+P_2 \rightarrow P_4$, $P_1+P_3 \rightarrow P_4$. The consumption term includes the reactions: $P_1+P_4 \rightarrow P_5$, $P_2+P_4 \rightarrow P_6$. Again, the application of the generalized balance equation should be obvious.

Cell culture population balance: (from biochemical engineering)

Cells grow in a Petri dish, a kind of batch reactor. These cells form clusters, much as in the polymer example. A two-cell cluster can be generated from 2 one-cell clusters. Two-cell and one-cell clusters can be consumed in the formation of a three-cell cluster. However, in addition to the terms in the polymer balance, equation (5), cells can be born and can die. Birth and death add terms to generation and consumption quantities of the balance. There are fancy models for cell birth and cell death, which a biochemical engineer would employ (but we will not).

The **cell cluster** balances for C_i, where i ranges from 1, 2, 3… to many million (i_{max}) are:

$$\begin{array}{ccccccc} \mathrm{acc} & = \mathrm{in} - \mathrm{out} + & \mathrm{gen} & - & \mathrm{con} \\ \dfrac{dC_i}{dt} & = 0 - \ \ 0 \ \ + & \left[\sum\limits_{j<i}^{i_{max}}\left(k_{j,i-j}C_jC_{i-j}\right) + \mathrm{birth}\right] & - & \left[\sum\limits_{j>i}^{i_{max}}\left(k_{i,j-i}C_iC_{j-i}\right) - \mathrm{death}\right] \end{array} \quad (6)$$

The application of the generalized balance equation should be obvious. No matter how convoluted the terms in the balance equation become, we should always be able to state specifically, whether a term belongs to the acc, in, out, gen, or con term. This should help us to make sure that every term we put in a balance equation belongs there as well as to make sure we get every term we need.

Human nation population balance: (from the social sciences)

The population of a country can be described with a balance equation. The in term is immigration. The out term is emigration. The generation term is birth rate. The consumption term is death rate.

The population balance for a country is then:

$$\begin{aligned} acc &= \quad in \quad - \quad out \quad + gen \quad - con \\ \frac{dPop}{dt} &= immigration - emigration + birth - death \end{aligned} \tag{7}$$

money balance: (from accounting)

The money in a bank account is subject to balance equations as well.

$$\begin{aligned} acc &= \quad in \quad - \quad out \quad + gen \quad - con \\ \frac{d\$}{dt} &= desposit - withdrawal + interest - 0 \end{aligned} \tag{8}$$

Enthalpy balance: (from thermodynamics)

Balance equation are constantly used to describe energy flow and generation of turbines, motors, reactors, boilers, and an endless list of other systems. There are many terms that can appear in the energy balance: heat can be generated by a reaction; heat can be removed by a cooling jacket; energy can flow in with the in stream or flow out in the exit stream; energy can be created by a change in volume, temperature, or pressure of the system; energy can be added to the system by mechanical work, like stirring, or it can be removed by doing work, as in the case of moving a piston in an engine. All these terms can appear in an energy balance but they will always be included in one of the acc, in, out, gen, or con quantities.

A typical **energy** balance, where H is some energy function and T is the temperature, for a combustion engine is:

$$\begin{aligned} acc &= \quad in \quad - \quad out \quad + \quad gen \quad - \quad con \\ \frac{dH}{dt} &= H_{in}(T_{in}) - H_{out}(T_{out}) + \text{Heat of reaction} - \text{work done} \end{aligned} \tag{9}$$

Mechanical Energy Balance: (from fluid flow)

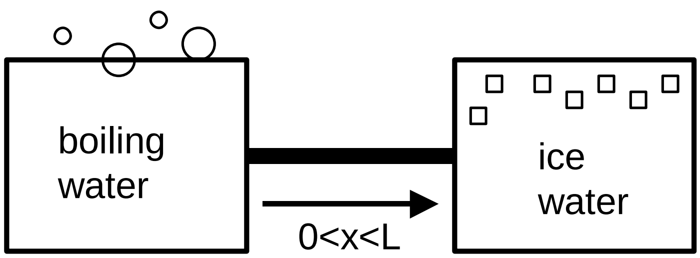
In this course, we will make balance equations of mechanical energy. The terms of the mechanical energy balance may include kinetic energy, KE, , potential energy, PE, , hydrostatic pressure head, ρgH, and a variety of frictional head losses, Σh_f. The kinetic energy, potential energy, hydrostatic pressure head are terms defined at the inlet and outlet, so they appear in both the in and out terms of the generalized balance equation. The frictional head loss terms are considered loss or consumption terms of the mechanical energy balance. The general mechanical energy balance for flow in a pipe, or flow out of a tank, etc. is:

$$
\begin{array}{llllll}
acc = & in & - \; out & + gen & - \; con \\
\dfrac{dE}{dt} & = (KE + PE + \rho g H)_{in} & - (KE + PE + \rho g H)_{out} & + 0 & - \sum h_f
\end{array}
\tag{10}
$$

The application of the generalized balance equation should be obvious. In this course, we will discuss the functional forms of the various terms in the balance.

Heat Balance: (from heat transfer)

In this course, we will make balance equations of heat (internal energy of translation, rotation, and vibration of molecules). If we place a heat conductor, like a metal rod, between a hot source, like a pot of boiling water, and a cold source, like a bucket of ice water, heat travels down the rod from the hot to the cold water.



This conduction of heat, Q, can be described at a point x along the rod by a balance equation in terms of the temperature, T.

$$
\begin{array}{llllll}
acc & = in & - \; out & + gen & - \; con \\
\rho C_p \dfrac{\partial T(x,t)}{\partial t} & = -k \dfrac{Q(x_{in},t)}{\Delta x} & - \; -k \dfrac{Q(x_{out},t)}{\Delta x} & + 0 & - \; 0
\end{array}
\tag{11}
$$

The application of the generalized balance equation should be obvious. In this course, we will discuss the functional forms of the various terms in the balance.

Entropy balance: (from thermodynamics)

Entropy, S, a thermodynamic measure of the disorder of a system, is also subject to the balance equation.

$$
\begin{array}{llllll}
acc = & in & - \; out & + \; gen & - \; con \\
\dfrac{dS}{dt} & = S_{in} & - \; S_{out} & + \; S_{gen} & - \; 0
\end{array}
\tag{12}
$$

Entropy has the additional constraint that there is never any consumption of entropy.

Momentum balance: (from fluid flow, transport phenomena)

Momentum, $\vec{p}$, the product of mass, m, and velocity, $\vec{v}$, is described by balance equations all the time. The equations that chemical engineers use to describe fluid dynamics are derived from momentum balances. These balances have some tricky terms since momentum is a vector quantity. However, these terms, as nasty as they can get, yield balance equations just like the ones we have shown above.

The most common momentum balance is Newton's second law, which we usually refer to as force equals mass times acceleration,

$$\vec{F} = m\vec{a} \tag{13}$$

However, we know that the acceleration is the time derivative of the velocity,

$$\vec{a} = \frac{d\vec{v}}{dt} \tag{14}$$

so that equation (15) becomes

$$\vec{F} = m\vec{a} = m\frac{d\vec{v}}{dt} = \frac{d(m\vec{v})}{dt} = \frac{d\vec{p}}{dt} \tag{15}$$

which can be rearranged to yield

$$\begin{array}{lcl} acc = & in - out + gen - con \\ \dfrac{d\vec{p}}{dt} = & F \end{array} \tag{16}$$

where the force, F, is an implicit summation of all the in, out, gen, and con momentum terms.

III. SOLUTION METHODOLOGY

From the examples given in the above section, we see that all balance equations take one of three forms:

- algebraic equation (usually from steady-state when the accumulation term is zero)
- ordinary differential equation, ODE, (usually for transient (non-steady state behavior)
- partial differential equation, PDE, (when a property varies with both position and time)

In order to solve the balance equations, we must know how to solve these three sorts of equations. In time past, engineering education was devoted in equal parts to (a) studying the fundamentals of engineering and (b) figuring out to solve the resulting equations.

From this perspective, the study of chemical engineering has become easier with time. With the advent of fast and widely accessible computers, the second task, that of figuring out how to solve the equations, has become almost trivial. At the University of Tennessee, we employ a software tool called MATLAB. Other software tools exist and they perform the same functions, albeit with differing syntax. However, the point is this: armed with a tool like MATLAB, the solution of algebraic equations, ODEs, and PDEs becomes almost trivial. There are packaged routines that will chug out the answer in no time flat.

This technology benefits us in several ways. First, it allows us to devote more time to understanding the fundamentals of the system. Second, it allows us to explore in greater depth than was previously possible the behavior of a system. Third, it empowers us as engineers to the point where we can say, "If I can write the balance equation, I can solve the problem." This is a very powerful statement and one which you should feel confident making at the conclusion of your studies in the Chemical Engineering Department.

This technology also presents some hazards. There is the saying about computer programs, "Garbage in, garbage out." If you don't understand how BOTH the physical system and the computer program work, you will not get reasonable solutions. Second, there is the danger of data-overload. Computers can generate a horrendous amount of data. It takes some measure of engineering skill to analyze the data, pick out the important stuff, relate the data to the physical system, and delete the rest of it.

Through-out this course, when the need arises, we will dedicate time to showing how we can use MATLAB to solve the systems of algebraic equations, ODEs, and PDEs that contain our balance equations.

IV. CONCLUSIONS

The key points to be drawn from this document are:

- balance equations provide a general, methodical technique for describing systems
- balance equations are the single-most powerful tool of the chemical engineer
- balance equations work for simple and extremely complex systems
- balance equations can be applied to volume, mass, moles, atoms, polymers, cells, people, money, enthalpy, entropy, mechanical energy, momentum, and just about anything else we can think of
- every class in the chemical engineering curriculum that follows ChE 200 and ChE 240 will use balances and will rely on your having mastered them in these courses
- you will be amazed at how much chemical engineering you can do once you master the use of balance equations
- A tool like MATLAB will make the solutions of our balance equations routine
- MOST IMPORTANTLY:

THE BALANCE EQUATION

$$\text{accumulation} = \text{in} - \text{out} + \text{generation} - \text{consumption}$$