1. OUTLINE AND MOTIVATION

1.1. The definition of the terms analysis and model

Let’s start out our subject by giving the dictionary definitions for the two terms we will be using frequently in this course, namely, analysis and model. The partial definitions for these terms relevant to our discussion are provided in Table 1.

**Table 1 Dictionary definitions for analysis and model**

<table>
<thead>
<tr>
<th>Analysis</th>
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<tbody>
<tr>
<td>1. The separation of an intellectual or material whole into its constituent parts for individual study.</td>
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<tr>
<td>2. The study of such constituent parts and their interrelationships in making up a whole.</td>
</tr>
<tr>
<td>3. A spoken or written presentation of such study: published an analysis of poetic meter.</td>
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<table>
<thead>
<tr>
<th>Model</th>
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</thead>
<tbody>
<tr>
<td>1. A small object, usually built to scale, that represents in detail another, often larger object.</td>
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<tr>
<td>2. A schematic description of a system, theory, or phenomenon that accounts for its known or inferred properties and may be used for further study of its characteristics: a model of generative grammar; a model of an atom; an economic model.</td>
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</table>

*Both definitions are abbreviated from Dictionary.com (Lexico, LLC 2001).*

In a broad sense, analysis is the sum of all acts performed for understanding a complex subject by dividing it into manageable chunks. The aim of a model is also to understand a complex subject. This tool achieves this goal by mimicking a relevant part of the real world. A road or geological map mimics earth’s surface. A wire mesh with plastic balls in the corners may be used to mimic the atoms in a crystal lattice. In the same sense, a set of mathematical relations can be used to mimic the behavior of a physical or chemical phenomenon.

Himmelblau and Bischoff gives us a complete definition for process analysis relevant to chemical engineering (Himmelblau, D. M. and Bischoff, K. B. 1968). In their approach, process analysis is referred to the application of scientific methods to the recognition and definition of problems. They also include the development of procedures for the solution of these defined problems into the general scheme of process analysis. In summary, in their view, process analysis involves an examination of the overall process, alternative processes and economics by

1. mathematical specification of the problem for the given physical situation,
2. detailed analysis to obtain the governing set of relations in the process,
3. synthesis and presentation of results to ensure full comprehension.

Chemical engineering profession, hence this course, deals with model types that are mathematical in nature. As it is apparent from Himmelblau and Bischoff’s definition above, mathematical modeling constitutes an integral part of the chemical engineering process analysis. Being proficient in process...
analysis requires a thorough understanding of mathematical modeling techniques. Before we begin with mathematical modeling techniques next chapter will provide a review of mathematical concepts necessary for various analysis and modeling techniques that are commonly used in chemical engineering.

The next section introduces the different uses of mathematical models in the broad concept of process analysis.

1.2. The uses and benefits of mathematical modeling of chemical processes

Chemical process industry stands out as a capital intensive industry with many subcomponents (Himmelblau, D. M. and Bischoff, K. B. 1968). Mathematical models enable us to analyze these subcomponents, hence the overall chemical process system at hand, in a structured and controlled way. It also minimizes the economic and safety risks inherent to the process.

Once there is a satisfactory mathematical model for a desired chemical process system, it can be used for different goals. These goals can be grouped under the following headings:

1. **Economics.** Capital cost estimation, selection between different alternative processes, product price determination.
2. **Design.** Size and type selection of processing equipment.
3. **Synthesis.** Selection of processing equipment and unit operation paths for optimum production levels with minimum cost.
4. **Control.** Keeping the processing equipments within the operational limits and the products within the customer specifications.
5. **Reliability.** Analyzing the effects of processing equipment failures on overall processing goals.
6. **Environment.** Analyzing the effects of chemical processes on the environment.

Before we proceed let’s appreciate the breadth of applications a chemical engineer can come across in his or her profession.

1.3. Breadth and depth of chemical engineering

By applying the same fundamental principles and similar concepts of momentum, heat and mass transfer and reaction kinetics, chemical engineers are able to deal with a wide range of problems in the engineering science. In its nature chemical engineering is very open to interdisciplinary industrial applications and research opportunities. It is common for chemical engineers to collaborate with electrical engineers in the microelectronics industry and materials science, with medical personnel, biologists and chemists in the pharmaceutical industry and with mechanical engineers in thermodynamics and heat transfer problems.

Russell and Denn discusses the variety of chemical engineering applications in light of three distinctly different chemical process systems (Russell, T. W. F. and Denn, M. M. 1972). Their first example is a chemical process for monoethylene glycol production. The second example is a secondary treatment unit for domestic sewage. Their final example is a device to be used as an artificial kidney.

1.3.1. Production of monoethylene glycol
A chemical process is to be developed where monoethylene glycol is produced with a 100 million pounds/year target. The selected process alternative is the hydration reaction of ethylene oxide. Their proposed processing scheme includes one reactor, two separators and one distillation column. The hydration reaction of ethylene oxide is as follows

$$H_2COCH_2 + HOH \rightarrow CH_2OHCH_2OH$$

The following reactions also occur in the reactor producing diethylene glycol and triethylene glycol as by-products.

$$CH_2OHCH_2OH + (CH_2)^2O \rightarrow CH_2OHCH_2OCH_2CH_2OH$$

$$CH_2OHCH_2OCH_2CH_2OH + (CH_2)^2O \rightarrow CH_2OHCH_2OCH_2CH_2OCH_2CH_2OH$$

Note that water boils at 100 °C whereas all the glycols boil at temperatures greater than 197 °C. For more details please refer to the listed reference (Russell, T. W. F. and Denn, M. M. 1972).

**Q.1.1** What are the functions of the four processing units?

**Q.1.2** What other processing units may be included to complete a more detailed analysis?

**Q.1.3** What kind of questions can be answered with the help of a mathematical model adequately describing the process?

### 1.3.2. Secondary treatment unit for domestic sewage

60 million gallons/day domestic sewage has to be treated so it can be discharged safely into natural water. A typical reactor for this process is an open tank with air sparging from bottom.

The design methods for this problem involves the biological oxygen demand (BOD) of the stream that needs to be treated. BOD is an overall measure of the oxygen amount to convert the organic mater in the sewage into H2O and CO2 in a batch laboratory reactor over a five day period. For more details please refer to the listed reference (Russell, T. W. F. and Denn, M. M. 1972).

**Q.1.4** What are the major similarities and differences between this process and monoethylene glycol production?

**Q.1.5** What kind of simplifications are brought to the analysis by the use of BOD?

**Q.1.6** What kind of questions can be answered with the help of a mathematical model adequately describing the process?

### 1.3.3. Artificial kidney

One of the functions of human kidney is the removal of metabolic waste products and poisons from the body. In this sense it resembles to a separation unit of chemical process systems. Although this is an oversimplification of the human kidney, with this analogy (model) relevant chemical engineering concepts can be applied for designing a device to replace certain functions of this vital organ. For more details please refer to the listed reference (Russell, T. W. F. and Denn, M. M. 1972).

**Q.1.7** What other subject areas would this design touch? Why?
Q.1.8 What are the major similarities and differences between this process and the first two processes discussed?

1.4. A simple process analysis and modeling exercise

The analysis of chemical engineering problems starts with a qualitative description of the problem. In this step, a schematic of the system is the most compact way of representing the physical situation. The schematic should include the known and unknown quantities with their respective units, important physical constants and a summary of major assumptions that might affect the subsequent steps. In the second step, the schematic is translated into mathematical language. All the relevant chemical and physical principles are identified and their relations are expressed to describe the mathematical model of the system. The third step involves the selection of a solution method that is applicable to the developed mathematical model in the previous step. The fourth step is the actual solution of the problem. The fifth step makes a reality check for the obtained solution and validates it. The final step presents the final results in a concise report.

The outlined steps in the previous paragraph will be applied to a simple system now. The system consists of an open tank filled initially with a constant density liquid. There is an orifice at the bottom of the tank for drainage. The system’s dynamic behavior is to be determined. The details of this system can be explored in the following reference (Russell, T. W. F. and Denn, M. M. 1972).

Step I. Schematic description of the problem

Figure 1 Schematic for the tank draining example

Step II. Building the mathematical model

In later chapters we will discuss the conservation equations in a structured fashion. However, this problem is simple enough to intuitively develop the governing equations for it. As there is no inflow to the tank, the conservation of mass requires that the rate of mass flow through the orifice be equal to the rate of change of mass in the tank.

\[
\frac{\text{rate of change of mass in the tank}}{\text{mass in the tank}} = \frac{d(\rho Ah)}{dt}
\]  
(1.1)
By combining the equations 1.1 and 1.2 we have the first form of the mathematical model for our simple system.

\[
\frac{d(\rho Ah)}{dt} = -\rho q
\]  

(1.3)

The two assumptions about the liquid density and cross-sectional area allow us to express the model in a simpler form after dividing both sides of equation 1.3 by the constant density \(\rho\).

\[
A \frac{dh}{dt} = -q
\]  

(1.4)

Equation 1.4 contains two unknown quantities, the liquid height, \(h\) and the liquid flow rate out of the orifice, \(q\). As there are two unknowns and only one equation there has to be a second relation for this mathematical model to be solvable. This additional relationship, constitutive relationship, will tie the quantities \(h\) and \(q\) making the model solvable.

The pressure difference across the orifice is the driving force for the liquid flow. Therefore, without losing any generality we can safely postulate that \(q\) is a function of \(\Delta p\) or in mathematical symbols

\[
q = q(\Delta p)
\]  

(1.5)

If the tank is open to atmosphere \(\Delta p\) would be proportional to \(h\). In light of the last information we would equally expect \(q\) to be a function of \(h\).

\[
q = q(h)
\]  

(1.6)

The simplest functional form between \(q\) and \(h\) would be assuming \(q\) to be a constant, \(c\).

\[
q = c
\]  

(1.7)

In later sections we will question the validity of this relation and discuss other possibilities. With this simplistic assumption, the combination of equations 1.4 and 1.7 becomes a fully solvable mathematical model for the open tank system.

\[
\frac{dh}{dt} = -\frac{c}{A}
\]  

(1.8)

**Step III. Selecting a solution method**

Equation 1.8 is simple enough to warrant an analytical solution to the model.

**Step IV. Solving the mathematical model**

The analytical solution of the model involves the integration of both sides with respect to time, \(t\), between an arbitrary time range \(t_1\) to \(t_2\).

\[
\int_{t_1}^{t_2} \frac{dh}{dt} dt = -\frac{c}{A} \int_{t_1}^{t_2} dt
\]  

(1.9)
The integral of a derivative is the function evaluations at the end points. So the solution is

\[ h(t_2) - h(t_1) = -\frac{c}{A} (t_2 - t_1) \]  

(1.10)

If \( t_1 \) is the initial time, 0, and \( h(t_i) \) is the corresponding initial liquid height, \( h_0 \), equation 1.10 can be expressed as

\[ h = h_0 - \frac{c}{A} t \]  

(1.11)

With an algebraic manipulation, the liquid height, \( h \), can be described as in the following working equation of the mathematical model.

\[ h = h_0 \left( 1 - \frac{c}{Ah_0} t \right) \]  

(1.12)

**Step V. Validating the mathematical model**

Validation of a mathematical model usually involves checking the model's behavior with respect to existing or new experimental data. However, before any experimental study is started the model's behavior at the system bounds is essential. If these validation tests fail there is no point immediately pursuing further. Instead we should be checking the prior steps for any errors. If there are no errors in the calculations, next step is to check the assumptions and to find the applicability range of the assumptions.

**Checking the model at the system boundaries.**

At \( t=0 \) the tank is 100% full and \( h \) is equal \( h_0 \). As the tank will eventually drain, as time goes to infinity the tank will be 0% full and \( h \) should become 0. Substituting 0 for \( t \) in equation 1.12 produces \( h_0 \) for \( h \). However, as \( t \) goes to infinity \( h \) approaches to negative infinity. So, our model fails the test at the second system boundary.

As the calculations in the previous steps are very simple, we can easily verify that they are in fact correct. Next, we need to go over the assumptions we used during the solution of the mathematical model. The assumptions about constant area and density were given by the problem definition. They should be safe to use. However, a closer look at the third assumption that the flow out of the orifice is constant proves to be wrong. As said earlier the liquid head above the orifice is the driving force for the flow. Therefore, as the liquid level decreases the flow rate out of the orifice should also decrease. Naturally, when the tank is fully drained the flow will stop. We discovered that the mathematical model we developed is not applicable to the whole operation range of the physical system. At this moment we have two choices. First, we can refine the functional relationship between \( q \) and \( h \), and solve the model again. The other choice is to go ahead and perform the experiments to determine the model's applicability range. Let's opt the second path and determine in what range this mathematical model would be applicable.

Below are the results for a tank-emptying experiment. The tank and orifice diameters are 1.0 and 0.043 in, respectively. One run is performed and the results are tabulated in Table 2. According to the equation 1.12, a plot of \( h \) vs. \( t \) should exhibit a linear relation with intercept \( h_0 \) and slope \(-\frac{c}{A}\). First, \( h \) values are plotted versus the time values, \( t \), as blue dots in Figure 2. Previously, we found that the mathematical model is not applicable to the entire time scale. This fact is also apparent in the plot. It appears that the linear behavior holds only for small time values. With this observation we make the linear fit optimized for time values smaller than 35 s. shown by the green line in the plot. The model's parameter \(-\frac{c}{A}\) becomes -0.158 in/s as determined graphically from the slope of the green line. This mathematical model would produce only accurate results for times less than 35 s.
Table 2 The results of the tank experiment for three runs

<table>
<thead>
<tr>
<th>h, in</th>
<th>t, s</th>
<th>h, in</th>
<th>t, s</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>0.0</td>
<td>7</td>
<td>56.7</td>
</tr>
<tr>
<td>14</td>
<td>6.0</td>
<td>6</td>
<td>66.1</td>
</tr>
<tr>
<td>13</td>
<td>12.2</td>
<td>5</td>
<td>76.2</td>
</tr>
<tr>
<td>12</td>
<td>18.7</td>
<td>4</td>
<td>87.6</td>
</tr>
<tr>
<td>11</td>
<td>25.5</td>
<td>3</td>
<td>101.0</td>
</tr>
<tr>
<td>10</td>
<td>32.7</td>
<td>2</td>
<td>117.5</td>
</tr>
<tr>
<td>9</td>
<td>40.3</td>
<td>1</td>
<td>140.7</td>
</tr>
<tr>
<td>8</td>
<td>48.3</td>
<td></td>
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</tr>
</tbody>
</table>

Step VI. Presenting the results

The mathematical model for the open tank drainage system is found to be a linear function of time for times less than 35 s.

\[ h = h_0 \left(1 - \frac{c}{A} t\right), \quad \text{where} \quad \frac{c}{A} = 0.158 \ \text{in/s} \quad \text{for} \quad t < 35s \]  \hfill (1.13)

Q.1.9 What would be the mathematical model if the relation between \( q \) and \( h \) is assumed to be a linear one as \( q = b h \)?

Q.1.10 What would be the mathematical model if the relation between \( q \) and \( h \) is assumed to be a generalized version of the previous two expressions with \( q = k h^r \)? What can you say about the range of the power \( r \)?
1.5. Estimating the order of a process

The model discussed in detail in the previous section and the model asked in question Q.1.9 are both two special cases of a broader model mentioned in Q.1.10 where the flow through the orifice is represented by a power relation, \( q = k h^r \). For \( r=0 \), the generalized model reduces to the case discussed in detail with constant flow rate. For \( r=1 \), it reduces to the case asked in question Q.1.9 with linear flow rate. Therefore, it would be nice to find the most appropriate exponent \( r \) before analyzing the experimental data for different \( r \) values by trial and error. In processes where there is a power relation like \( q = k h^r \), the exponent \( r \) is said to be the order of the process. There is a standard technique for estimating this order from experimental data. After the exponent is determined, the mathematical model can be solved for the specific power relation of the process.

Estimating the order for the tank-emptying process will be described briefly now. The mathematical model for the system with the power relation opted for the flow rate \( q \) can be expressed as

\[
\frac{-dh}{dt} = \frac{k}{A} h^r
\]  

(1.14)

Taking the natural logarithms of both sides results in

\[
\ln\left(\frac{-dh}{dt}\right) = \ln\left(\frac{k}{A}\right) + r \ln h
\]  

(1.15)

The above equation defines a linear relation between \( \ln(-dh/dt) \) and \( \ln h \) with intersection \( \ln(k/A) \) and slope \( r \). Using this fact the order of the process, \( r \), can be estimated from a plot of \( \ln(-dh/dt) \) versus \( \ln h \) as the slope of the line.

If the experimental data is free of scatter, evenly spaced and error free, the described use of equation 1.15 would result in a good order estimate for the process. The reason for these limiting
conditions come from the fact that in the procedure of estimating the slope, the experimental data needs to be differentiated numerically. The original data consisted of \( h \) and \( t \) values. However, in the order estimation we are interested in \( \ln(-dh/dt) \) and \( \ln h \) values. The accuracy of numerical differentiation is known to be little. For data that obeys the mentioned limitations the method gives reasonable bounds for the process' order. However, it is not a good idea to use this method to estimate \( k \). The accuracy of the method is not great to start with and the natural logarithm would only magnify the effects.

Q.1.11 Find the order of the process using the original \( h \) vs. \( t \) data of the tank emptying experiment?

Q.1.12 Propose a complete model with corresponding \( k \) and \( r \) values that can explain the entire data range for the tank emptying experiment?

1.6. Discussion

Before we start a detailed analysis in the following chapters we tried to give a glimpse of a general process analysis and modeling exercise applied to a simple system. Although, each modeling problem will have its unique character and corresponding solution methods some of the ideas presented in this chapter are applicable universally. First, we need to appreciate the fact that the goal is to approximate a relevant feature of the real world. To isolate the relevant feature from the complexities of the real world is a difficult task in itself. Additional difficulties may arise in converting our perception of the relevant part of the world into mathematical language and propose a solution method for it.

In the previous example, we were fortunate to have a process where the order was possible to estimate with the help of nicely arranged experimental data. If order estimation was not possible, we had to guess the correct relation between \( q \) and \( h \) and estimate its parameters. As Russell points out, in general, this kind of unknown behavior in a modeling problem is the rule rather than the exception (Russell, T. W. F. and Denn, M. M. 1972). Therefore, it is not false to say that process analysis and modeling problems commonly have a controlled trial-and-error component in them.

Aris explains this fact in his book by describing the modeling task as a periodic oscillation between two levels, conceptual progress and actual understanding of a physical phenomenon, improving the overall model along the way (Aris, R. 1994). Aris' view is presented in Figure 3. In the oscillation between conceptual progress and actual understanding, elementary ideas lead to the first model. The first model's use generates experience. Finally, the experience enables the modeler to revise the initial ideas and assumptions which in effect leads to a better second model.

Aris also emphasizes in his book that the revision of ideas and a better understanding of the process do not necessarily mean a more complex model. A lot of the times a better understanding of the process can lead to simpler models with fewer parameters.
Figure 3 Aris’ view of the modeling process (adapted from (Aris, R. 1994))

References


