CHAPTER 8 ENTERING DIMENSIONAL EQUATIONS FROM HANDBOOKS

Often in creating an ASCEND model one needs to enter a correlation given in a handbook that is written in terms of variables expressed in specific units. In this chapter, we examine how to do this easily and correctly in a system like ASCEND where all equations must be dimensionally correct.

8.1 EXAMPLE 1— VAPOR PRESSURE

Our first example is the equation to express vapor pressure using an Antoine-like equation of the form:

$$\ln(P^{sat}) = A - \frac{B}{T + C} \quad \textbf{(8.1)}$$

where P^{sat} is in {atm} and T in {R}. When one encounters this equation in a handbook, one then finds tabulated values for A, B and C for different chemical species. The question we are addressing is:

How should the modeler enter this equation into ASCEND so he or she can then enter the constants A, B, and C with the exact values given in the handbook?

ASCEND uses SI units internally. Therefore, P would have the units {kg/m/s^2}, and T would have the units {K}.

Equation 8.1 is, in fact, dimensionally incorrect as written. We know how to use it, but ASCEND does not as ASCEND requires that we write dimensionally correct equations. For one thing, we can legitimately take the natural log *(ln)* only of unitless quantities. Also, the handbook will tabulate the values for A, B and C without units. If A is dimensionless, then B and C would require the dimensions of temperature.

The mindset to enter such equations is to make all quantities that must be expressed in particular units into dimensionless quantities which have the correct numerical value.

We illustrate in the following subsections just how to do this conversion. It proves to be very straight forward to do.

8.1.1 CONVERTING THE *LN* TERM

Convert the quantity within the *ln()* term into a dimensionless number that has the value of pressure when pressure is expressed in {atm}.

Very simply, we write

```
P_atm = P/1{atm};
```

Note that P_atm has to be a *dimensionless* quantity here.

We then rewrite the LHS of Equation 8.1 as

```
ln(P_atm)
```

Suppose P = 2 {atm}. In SI units P= 202,650 {kg/m/s^2}. In SI units, the dimensional constant 1{atm} is about 101,325 {kg/m/s^2}. Using this definition, P_atm has the value 2 and is dimensionless. ASCEND will not complain with P_atm as the argument of the *ln* () function, as it can take the natural log of the dimensionless quantity 2 without any difficulty.

8.1.2 CONVERTING THE RHS

We next convert the RHS of Equation 8.1, and it is equally as simple. Again, convert the temperature used in the RHS into:

```
T_R = T/1{R};
```

ASCEND converts the dimensional constant 1{R} into 0.55555555...{K}. Thus T_R is dimensionless but has the value that T would have if expressed in {R}.

8.1.3 IN SUMMARY FOR EXAMPLE 1

We do not need to introduce the intermediate dimensionless variables. Rather we can write:

```
ln(P/1{atm}) = A - B/(T/1{R} + C);
```

as a correct form for the dimensional equation. When we do it in this way, we can enter A, B and C as dimensionless quantities with the values exactly as tabulated.

8.2 FAHRENHEIT— VARIABLES WITH OFFSET

What if we write Equation 8.1 but the handbook says that T is in degrees Fahrenheit, i.e., in {F}? The conversion from {K} to {F} is

T{F} = T{K}*1.8 - 459.67

and the 459.67 is an *offset*. ASCEND does not support an offset for units conversion. We shall discuss the reasons for this apparent limitation in Section 8.4.

You can readily handle temperatures in {F} if you again think as we did above. The rule, even for units requiring an offset for conversion, remains: convert a dimensional variable into dimensionless one such that the dimensionless one has the proper value.

Define a new variable

```
T_degF = T/1{R} - 459.67;
```

Then code Equation 8.1 as

```
ln(P/1{atm}) = A - B/(T_degF + C);
```

when entering it into ASCEND. You will then enter constants A, B, and C as dimensionless quantities having the values exactly as tabulated. In this example we *must* create the intermediate variable T_degF.

8.3 EXAMPLE 3— PRESSURE DROP

From the Chemical Engineering Handbook by Perry and Chilton, Fifth Edition, McGraw-Hill, p10-33, we find the following correlation:

$$\Delta P'_a = \frac{y(V_g - V_l)G^2}{144g} \qquad \textbf{(8.2)}$$

where the pressure drop on the LHS is in psi, y is the fraction vapor by weight (i.e., dimensionless), Vg and V_l are the specific volumes of gas and liquid respectively in ft^3/lbm, G is the mass velocity in lbm/hr/ft^2 and g is the acceleration by gravity and equal to 4.18x10^8 ft/hr^2.

We proceed by making each term dimensionless and with the right numerical value for the units in which it is to be expressed. The following is the result. We do this by simply dividing each dimensional variable by the correct unit conversion factor.

```
delPa/1{psi} = y*(Vg-Vl)/1{ft^3/lbm}*
               (G/1{lbm/hr/ft^2})^2/(144*4.18e8);
```

8.4 THE DIFFICULTY OF HANDLING UNIT CONVERSIONS DEFINED WITH OFFSET

How do you convert temperature from Kelvin to centigrade? The ASCEND compiler encounters the following ASCEND statement:

```
d1T1 = d1T2 + a.Td[4];
```

and d1T1 is supposed to be reported in centigrade. We know that ASCEND stores termperatures in Kelvin {K}. We also know that one converts {K} to {C} with the following relationship

T{C} = T{K} - 273.15.

Now suppose d1T2 has the value 173.15 {K} and a.Td{4} has the value 500 {K}. What is d1T1 in {C}? It would appear to have the value 173.15+500-273.15 = 400 {C}. But what if the three variables here are really temperature differences? Then the conversion should be

T{dC} = T{dK}.

where we use the notation {dC} to be the units for temperature difference in centigrade and {dK} for differences in Kelvin. Then the correct answer is 173.15+500=673.15 {dC}.

Suppose d1T2 is a temperature and d1T2 is a temperature difference (which would indicate an unfortunate but allowable naming scheme by the creator of this statement). It turns out that a.Td[4] is then required to be a temperature and not a temperature difference for this equation to make sense. We discover that an equation that involves the sums and differences of temperature and temperature difference variables will have to have an equal number of positive and negative temperatures in it to make sense, with the remaining having to be temperature differences. Of course if the equation is a correlation, such may not be the case, as the person deriving the correlation is free to create an equation that “fits” the data without requiring the equation be dimensionally (and physically) reasonable.

We could create the above discussion just as easily in terms of pressure where we distinguish absolute from gauge pressures (e.g., {psia} vs. {psig}). We would find the need to introduce units {dpisa} and {dpsig} also.

8.4.1 GENERAL OFFSET AND DIFFERENCE UNITS

Unfortunately, we find we have to think much more generally than the above. Any unit conversion can be introduced both with and without offset. Suppose we have an equation which involves the sums and diffences of terms t1 to t4:

$$\mathbf{t1 + t2 - (t3 + t4) = 0} \qquad \textbf{(8.3)}$$

where the units for each term is some combination of basic units, e.g., {ft/s^2/R}. Let us call this combination {X} and add it to our set of allowable units, i.e., we define

{X} = {ft/s^2/R}.

Suppose we define units {Xoffset} to satisfy:

{Xoffset} = {X} - 10

as another set of units for our system. We will also have to introduce the concept of {dX} and and should probably introduce also {dXoffset} to our system, with these two obeying

{dXoffset} = {Xoffset}.

For what we might call a “well-posed” equation, we can argue that the coefficient of variables in units such as {Xoffset} have to add to zero with the remaining being in units of {dX} and {dXoffset}. Unfortunately, the authors of correlation equations are not forced to follow any such rule, so you can find many published correlations which make the most awful (and often unstated) assumptions about the units of the variables being correlated.

Will the typical modeler get this right? We suspect not. We would need a very large number of unit conversion combinations in both absolute, offset and relative units to accomodate this approach.

We suggest that our approach to use only absolute units with no offset is the least confusing for a user. Units conversion is then just multiplication by a factor both for absolute {X} and difference {dX} units— we do not have to introduce difference variables because we do not introduce offset units.

When users want offset units such as gauge pressure or Fahrenheit for temperature, they can use the conversion to dimensionless variables having the right value, using the style we introduced above, i.e.,

T_defF = T/1{R} - 459.67

and

P_psig = P/1{psi} - 14.696

as needed.

Both approaches to handling offset introduce undesirable and desirable characteristics to a modeling system. Neither allow the user to use units without thinking carefully. We voted for this form because of its much lower complexity.