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Documenting Process Calculations

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Documenting Process Calculations

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INTRODUCTION

At some point in most projects process calculations are produced. These calculations include various formulas, physical property data, equipment details, and equipment and piping layouts. Getting accurate physical property data and selecting the proper equations is critical to producing valid results and a workable design. The calculationsare critical in the future for verification of the process, for repairs to damaged systems and on occasion for legal problems.

Selecting valid equations is the basis of the engineer's education and experience and contains some latitude; for example there are multiple methods which can be used to calculate fluid pressure drops in pipe.

Selecting physical properties is an ongoing process as demanded by the work at hand; there are also multiple sources of physical property data and errors are a problem. With the advent of the Internet it is both easier and more difficult to get good data. Some data sources follow:

Manufacturer issued MSDS (Material Safety Data Sheet)
CRC Handbook
Perry's Chemical Engineer's Handbook
Crane 410
Multiple Internet sites
Most Internet search engines will bring up data based on entry of the chemical name

The final design package in the permanent files contains all of the drawings and should contain the original calculations. Some of the drawings will be stamped by a PE depending on state and client requirements. Likewise the calculations should be stamped by the engineer doing the calculations. For the calculations to serve all their purposes they should be completed in such a way as to provide proper documentation for the records.

DOCUMENTATION

Documentation is a term used in several different ways. Generally, documentation (to document) refers to the process of providing evidence.

The evidence to be provided with the equations used in the calculations should be sufficient to prove the selected equations are applicable to the problem being solved. Normally showing the equation and providing some reference to an accepted standard is all that is required.

The evidence to be provided with the physical property data is generally a reference to the source of the data. Normally an accepted standard like the CRC Handbooks, Perry's or a similar document is required along with page number and edition of the standard. For example Perry's 6^{th} ed. Table 1 page 453.

EQUATIONS FOR CALCULATIONS

Most engineers will use some accepted standard as a source for the various equations needed for calculations. This might be Perry's, Crane©410 or a similarly accepted document.

There are basically two types of equations in use in calculations:

Commonly known with no need for evidence such as:

1. The cross sectional area of flow for the pipe is calculated as: $A = \pi\ (ID/2)^2$

There is no need to reference the source of an equation in common usage such as the area of a circle or other simple geometric shape. It is enough that the object is defined in a recognizable manner along with the desired information such as area or volume.

2. The log mean temperature difference is calculated as:

   LMTD = (GTTD-LTTD)/(ln(GTTD/LTTD))

Not only is a reference required but in this case the definitions of GTTD and LTTD are required for further understanding about the calculation. Depending on the equipment the temperatures used may be selected differently. (Professional Publications "Chemical Engineering Reference Manual", 5^{th} Ed. Equation 7.25 page 7-7). On occasion a small sketch is the best definition as in this case.

CONSTANTS

Some equations contain standard constants examples follow:

π	pi	
g_c	gravitational constant,	32.174 lb_m-ft/lb_f-sec^2
G	gravitational constant,	3.44×10^{-8} ft^4/lbm-sec^4
R	Universal gas constant	1545 ft-lb_f/lb_{mol}-°R

Most of these are commonly used and do not require explanation but inserting units keeps the math straight.

ABBREVIATION OF UNITS / FUNCTIONS

The units assigned to various numbers can cause errors if misinterpreted. Some abbreviations occur in multiple disciplines and have widely differing meanings.

Viscosity	centipoise	cps	in electrical this is cycles per second

	centipoise Cp	this is also specific heat
Specific Heats	constant pressure	Cp
	constant volume	Cv also can be Flow Coefficient
Ln	Natural log, base e	
Log	Base 10 log	
Psia	Pressure, absolute, Psig + 14.7	
Psig	Pressure, gage	

SYMBOLS

°	Degrees (Rankine, Centigrade, Fahrenheit), angular degrees
^	Exponent, Power
X or *	Multiplication
/ or ÷	Division
+	Addition

Most of these are explained by the context of the equation and are common enough not to required either definition or reference..

GREEK LETTERS

Greek letters are commonly used in engineering equations across all disciplines, where the meaning is not obvious from assigned units or the equation in question they should be defined.

ρ	Density
μ	Absolute viscosity
Δ	Difference
λ	Heat of vaporization
ε	Absolute pipe roughness
β	Ratio of diameters

Crane© 410 25th Edition, first page.

SUBSCRIPTS

Frequently equations contain the same letter with subscripts, if not clear from the equations or sketch on the calculation sheet then definition is required. Example:

D_1	Possibly upstream diameter or larger diameter
D_2	Possibly downstream diameter or smaller diameter
P_1	Inlet pressure

P_2 Outlet pressure

CONVERSIONS

Frequently a calculation starts in one set of units and finishes in a different set, US to metric and ft^3 to gallons being examples.

50 gpm = 6.68 ft^3 / min
50 gpm = 3.15 liters / sec

Generally as long as all the numbers (50, 6.68 and 3.15 above) have the correct units no explanation or reference is required. Unusual units deserve definition, for example Barrels works well and doesn't require definition in an oil field calculation but would need definition in a specialty chemical or pharmaceutical plant.

A LOOK AT INTERNET CALCULATIONS

Many process engineers do calculations using freely downloaded software, a web site for the calculations or purchased software. All of these methods share several documentation drawbacks as will be seen in the following example of calculating fluid flow pressure drops:

- You generally cannot see the mathematical operations being performed
- It may be difficult to verify the "library" data the software uses.
    - physical properties (viscosity, density, etc.)
    - pipe dimensions, schedules, roughness, etc.
- It may be difficult to verify the equations used and their applicability to your specific problem
    - calculated "f" values
    - compressible verses non-compressible flow
    - pipe lines verses short pipe runs
    - etc.
- If your particular fluid or pipe material is not in the software library it may be difficult to add data for them
- Most of the downloaded material does not consider mechanical tubing (as frequently used in the pharmaceutical industry) as "pipe" so the dimensions are not in the libraries; the same is frequently true for copper and stainless tubing frequently used in tracing, catalyst and low flow systems
- You may not be able to add in "equivalent lengths" ("K" values) for nonstandard equipment or piping components (slide valves, coils, strainers, etc)
- The data input units may require you to convert from your normally used facility units (gpm. lpm, m^3/s, etc) to some other units
- In some cases a stamped copy of the calculations is required for the files or client; an adequate copy would show what the software is doing or give some indication that the

software has been validated. Validation of downloaded software may be difficult to obtain.

- Printing the calculation output page does not usually show any of the math used.

Regardless of the source the PE using the software remains responsible for the results of the calculations. That means at times the calculations must be done in detail by the engineer, it frequently means that using downloaded or net based software isn't going to produce the desired file copies of the calculations. More often than not the only output of net based work is a single page with the results of the calculations as follows.

Pressure Drop Online-Calculator

Calculation output

Flow medium:	Water 20 °C / liquid
Volume flow::	50 gal/min
Weight density:	62.318 lb./cu.ft.
Dynamic Viscosity:	1.0762cP
Element of pipe:	circular
Dimensions of element:	Diameter of pipe D: 2.067 in.
	Length of pipe L: 100 ft.
Velocity of flow:	4.78 ft./s
Reynolds number:	76467
Velocity of flow 2:	-
Reynolds number 2:	-
Flow:	turbulent
Absolute roughness:	.00015 in.
Pipe friction number:	0.02
Resistance coefficient:	11.24
Resist.coeff.branching pipe:	-
Press.dropbranch.pipe:	-
Pressure drop:	249.18 lbw./sq.ft.
	1.75 psi

Note: The pressure drop was calculated by the online calculator of www.pressure-drop.com. We can not warrant the correctness of this software. The software is produced carefully. But no computer software is without bugs. Therefore the calculations are your own risk.
****

Do you know our software SF Pressure Drop 7.x for Windows?
Information: www.pressure-drop.com
www.**pressure-drop**.com/Online-Calculator/index.htm

Crane 410© page B-14 reports the following for the same conditions given above:

Velocity	4.78 ft/sec
Pressure drop	2.03 psi

Difference = 100 x [(2.03-1.75)/2.03] = 13.8%

The pressure drop is shown as 1.75 psi which was converted from 249.18 lbw./sq.ft. whereas the result of the conversion actually should be 1.73 psi. A small error (1.1%) but one which indicates a problem within the software.

Note that no equations are given and the size of the difference from an accepted standard is sufficiently large that most engineers would not use the value. Also note the disclaimer accompanying the results which indicates un-validated software. It is possible to validate the software off line but the effort is significant and subject to change when the software is changed by the web site. In reality the software would require re-validation prior to each use since no notice of change is presented. No documentation is provided by the results page of the calculations.

The engineer using these results would, under some conditions, be required to place his stamp on the calculations.

Classical sources of equations have been used for years and generally include the engineer's text books as well as standard reference books for his / her discipline (ig. Perry's Chemical Engineer's Handbook). A properly documented formula on a page of calculations would take a format similar to the following:

Calculate Reynolds Number

$N_{Re} = \frac{DV\rho}{\mu}$ Crane© 410 page 3-2

On occasion it may be necessary to define terms within the equation, for example:

$N_{Re} = \frac{B\rho}{d\mu}$ Crane© 410 page 3-2

B = rate of flow in Barrels per hour

Fluid velocity = flow rate divided by cross sectional area of the pipe; from the example above:

50 gpm = 6.68 ft^3/min
Pipe ID = 2.067, cross sectional area = .0233 ft^2
Velocity V = 6.68ft^3/min ÷ 0.0233 ft^2 x min/60 sec = 4.78 ft./sec.

Although the math was performed to calculate the flow area in square feet from the diameter in inches the inclusion of a basic math formula for this kind of calculation is not needed since the verbiage explains what has been done and enough detail is present to allow someone to check the result.

Note that units are provided for each numerical value; this is also essential to complete documentation for the math. Numbers which should have units but do not have no meaning in calculations. Some units are given as initials(gpm, ft.) as these are recognized standard abbreviations. However, in the sample the abbreviation cPfor centipoise is not so well known and exists also as cps; some explanation is required in cases where confusion might exist. Remember the goal of documentation is to make the calculations clear and verifiable.

When purchased or validated down loaded software is used it should be referenced:

Crane 410-TP "Flow of Fluids Premium", Version 1.0

The sample software fails to document the calculations in any fashion. There is no way for anyone to verify any of the math used nor verify the results unless they run the calculations separately which sort of defeats the use of the web software to begin with.

PHYSICAL PROPERTY DATA

Two problems are encountered when searching for physical property data:

Finding valid data
Finding data at the points involved in the project

One of the items in an engineering calculation that requires documentation is the physical data used in the calculations. Rarely does the process point (temperature, pressure, etc.) match the available data points provided with the physical property data. Still we need to use the data in the calculations and we need to document the validity of the data point.

Working from tabulations found in accepted standards and using math to find the data at our required process point is acceptable as long as the math used is valid. We'll look at the first section and try to produce some comparisons.

INTERPOLATION -AT THE EXACT POINT

More often than not I need the data at points not listed in tabulations. But a tabulation allows me to interpolate to the point I need. Probably the most common interpolations occur with steam tables. We'll use a portion of the steam tables from Crane© 410 as one of our examples in this material.

The ease with which interpolations can be accomplished tends to make me want to make the task even easier. The first step was to set up a simple interpolation function in an Excel™ spread sheet and enter data from a tabulation rather than doing any calculations myself.

Why not utilize one of the spread sheets and set up functions to provide the desired information with a simple pressure or temperature point input. This worked using an Excel™ "lookup" function and simplified the task even further.

That worked so well that I decided that once the data points were in the spread sheet it would be an easy matter to insert trend lines of the data into a data graph. With most spread sheets the trend line equation is presented. From this equation it was a simple matter to produce a simplified spread sheet which would calculate the desired data at any temperature or pressure. A comparison plot of real data points from a tabulation using Excel™ produced a trend line which was visually identical to the original data curve.

If it was that easy it would have been done before. It was that easy, trouble was that the errors in the trend line equation were significant and that's why it isn't done the easy way. Trend lines generally do not make valid documentation.

Interpolation works when the graph of the line between the interpolation points is straight. For example in the following interpolation of steam data we are in a section of the temperature verses pressure curve which is relatively straight. Other curves, benzene vapor pressure verses temperature, have a significant curve at low pressures and a relatively straight portion at higher pressures. The relative errors indicate the absolute necessity of examination of the data prior to using interpolated data as documentation for calculations.

EXAMPLE 1 INTERPOLATION

Interpolation essentially assumes that the data changes from one point to the next in a straight line. This is generally true if the interval between points is sufficiently small. Consider the following points from the steam tables:

Pressure	Temperature	Interpol-ation between	Range Between Points	Interpolated Value for Midpoint	Error = (Table Value minus Interpolated Value)x100/(Table Value)
psia	^oF		psi	^oF	%
100	327.82	X	2	328.54	0.00%
101	328.54				
102	329.26	X			

100	327.82	X			
102	329.26		4	329.25	0.00%
104	330.67	X			
100	327.82	X			
104	330.67		8	330.63	0.01%
108	333.44	X			
100	327.82	X			
110	334.79		20	334.55	0.07%
120	341.27	X			
100	327.82	X			
125	344.35		50	343.13	0.35%
150	358.43	X			
100	327.82	X			
150	358.43		100	354.81	1.01%
200	381.80	X			
100	327.82	X			
200	381.80		200	372.59	2.41%
300	417.35	X			
100	327.82	X			
300	417.35		400	397.42	4.78%
500	467.01	X			
100	327.82	X			
350	431.70		500	407.01	5.72%
600	467.01	X			

It would appear that interpolation of values within THIS SEGMENT of the steam tables for a range as wide as 400 psi still provides values which would allow for plus or minus 5% accuracy in engineering calculations.

Documentation of interpolated data is important and should take a format similar to the following.

Steam pressure 305 psia Temperature = 418.84 °F
Straight line interpolation 300 to 320 psiaCrane ©410 page A-15

An assumption that this level of accuracy carries over to other tabulations of physical properties and for materials other than steam is most likely not a good idea. Each tabulation needs to be checked for accuracy of interpolations to verify the allowable range over which the straight line assumption mathematics is valid.

As an example of errors generated by interpolating the vapor pressure of benzene shows unacceptably large errors for the interpolated value. Even with relatively small differences between the interpolation points the error is still outside acceptable limits.

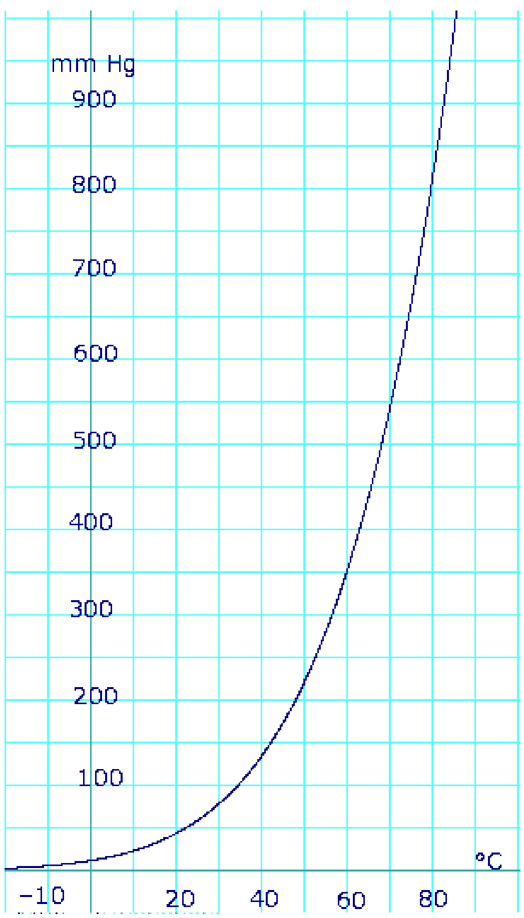
Basis: Benzene, C_6H_6, Wikipedia (Table data obtained from *CRC Handbook of Chemistry and Physics* 44th ed)

Vapor Pressure	Temperature	Interpol-ation between	Range Between Points	Interpolated Value for Midpoint	Error = (Table Value – Interpolated Value)/Table Value
psia	^oF		psi	^oF	%
0.02	-34.06	X			
0.19	11.30		0.75	18.46	-63.36%
0.77	45.68	X			
0.19	11.30	X			
0.77	45.68		1.74	33.86	25.88%
1.93	78.98	X			
0.77	45.68	X			
1.93	78.98		6.95	61.58	22.03%
7.72	141.08	X			
1.93	78.98	X			
7.72	141.08		12.74	123.16	12.70%
14.67	176.18	X			
7.72	141.08	X	21.62	166.07	5.74%

14.67	176.18				
29.34	218.84	X			
14.67	176.18	X			
29.34	218.84		58.67	204.26	6.66%
73.34	288.50	X			

A graph of the data which shows as a curve is an indication that straight line interpolation is not a valid approach to obtain data between known points in the lower temperature range.

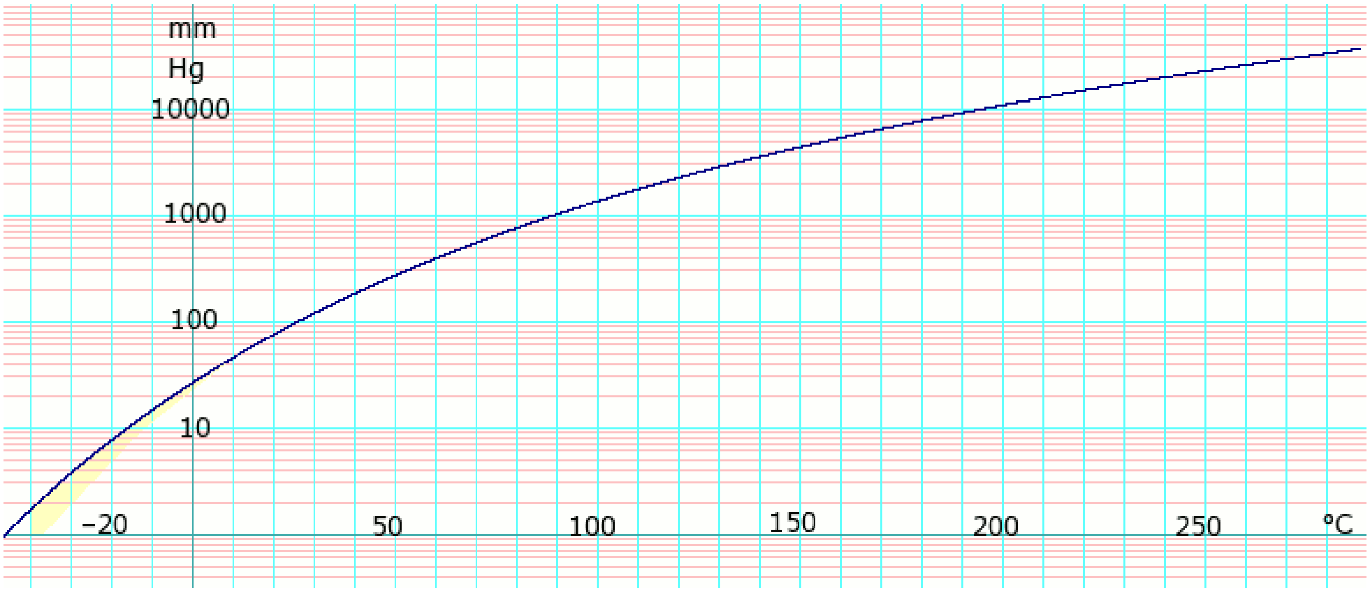
CH3CH2OH Vapor Pressure



In the vapor pressure curve for ethanol above note that the extreme curve up to about 50°C is too severe for straight line interpolation. A curve using a parabolic function could be used fromabout -10 to 50°C for interpolation when the effort is worth the time it would take.

GRAPHICAL

Occasionally the only form in which data is available is graphical; although less convenient than a tabulation the graph is still sufficient for documentation purposes. The following log-log graph covers the same data as the tabulation of the vapor pressure of benzene above.



Where the tabulation allows us to read the vapor pressure and temperature to two decimals the graphical representation is essentially limited to a guess for the second and third digits. For example consider the following:

	Vapor Pressure mmHg / psia	Temperature °C / °F
Tabulation	760 / 14.67	80 / 176.18
Graph	750 psia	80°C

The 80°C happens to be an easily read vertical line on the graph but the 750 mm Hg is a guess as to the last two digits (50) part of the reading. Although valid data, the accuracy for this particular graph is considerably less than for the tabulation. Attempting to read the graph for a temperature of 76°C requires a guess for both the temperature and pressure.

Utilizing this graph as the source of the data for calculations introduces some error compared with the tabulation but when it is the only source of data there isn't much choice. Documentation should list the graph and its source or can be an attachment containing the graph.

EQUATIONS OF STATE

A search will yield a variety of Equations of State for various chemicals and various properties, we take two equations and compare two properties to the other data from more typical sources, we'll stay with ethanol.

One of the more common is the Clausius-Clapeyron series of equations, see References.

The Clausius–Clapeyron equation determines the vapor pressure $P$of a liquid as a function of temperature T(in degrees K). Improved accuracy can be obtained using the Antoine equation $\log_{10} p = A - \frac{B}{C+T}$, where A, B, $C$are empirical constants for each substance.

"Clausius-Clapeyron Equation for Some Common Liquids" from the Wolfram Demonstrations Projecthttp://demonstrations.wolfram.com/ClausiusClapeyronEquationForSomeCommonLiquids/

Vapor Pressure

$Log_{10}(p) = A - (B/(C+T))$
P = Vapor pressure, mmHg
A = 18.8119
B = 3803.98
C = -41.68
T = 20 °C = 20 + 273.16 = 293.16K

And

Viscosity

Log(v) = B*(1/T-1/C)
V = viscositycps
B = 686.64
C = 300.88
T = 293.16 K

See results in tabulation below. For ethanol,CH_3CH_2OH,we’ll use CRC data as the correct value.

FINAL RESULTS

We can now compare the data search as shown in the table below.

Source	Temperature °C	Density, #/ft3	Viscosity, cps	% Error Viscosity	Vapor Pressure, psi	% Error, Vapor Press.
Crane© 410	20 C		1.25 (G)	0.83		
Perry’s	20 C	49.23 (T)	1.19 (G)	0.00	0.827 (IT)	2.13
CRC 40th Edition	20 C	49.26 (T)	1.20 (T)	0.00	0.845 (IT)	0.00
MSDS, (Fisher)	20 C	49.23 (L)	1.20 (L)	0.00	0.862 (L)	-2.01
Wikipedia	20 C	49.26	1.2 (L)	0.00	0.862 (L)	-2.01

		(L)				
Internet Search	20C	49.23 (L)	1.20 (T)	0.00	0.946 (G)	-11.95
EOS, Clausius-Clapeyron	20C		1.14 (EOS)	5.00	0.7694 (EOS)	8.94

T = Tabulation, L = List, G = Graph, IT = Interpolated Tabulation, EOS = Equation of State

All of the above except the MSDS, the Internet search and some EOS equationsare considered accepted standards and the differences between data values are minimal. This Wikipedia data is from a CRC tabulation. In the case of Wikipedia if there is no reference to another standard using that as documentation or a source is not a good plan.

Gas densities are generally reported at STP (Standard Temperature and Pressure) Sometimes one data point comes from one source and the next from a different source. There is nothing wrong with using two different sources as long as they are "standards." For example using the nitrogen density at 68°F and 14.7 psia from Crane© 410 and the nitrogen density at 100°F and 14.7 psia from Perry's for interpolation to find the density at 80°F. In the documentation just list both.

CALCULATION LAYOUT

The page layout for calculations is a choice of the engineer but should follow some logical progression with notes included where appropriate. Neatness counts and sloppiness counts against.

Properly erasing mistakes so the new work is clear and clean is important. Nothing makes others more suspicious of the calculations than a smudged or questionable number. Some engineers line through mistakes rather than erase. For future reference (particularly in court cases) the engineer can initial and date the line through; this action removes doubt later as to when the correction was made. "Pressure is ~~15 psig~~ 150 psig." Squeezing in the needed "0" makes the work look sloppy. CW 3/12/2011

All calculation and all pages should contain at a minimum the following:

- Engineer's name
- Engineer's stamp, signed and dated
- Date of calculations
- Equipment or process name
- Calculation Basis
- Project number if applicable
- Client name
- Page numbers
- Purpose of calculations

This latter item is critical since it establishes the base line for the calculations. For example in heat transfer calculations the Basis provides the material being heated and its physical properties, the heating medium, the time line and the desired goal for temperature and pressure. Putting the basis at the beginning of the calculations allows a future reader to understand the path of the calculations before getting into the calculations. Remember the purpose of documentation is to ensure proper understanding.

If a peer review of the calculations is performed then the reviewer's name and date of review should be included.

CONCLUSION

Calculations serve an immediate purpose: equipment sizing, pipe sizing and utility loads. Future purposes include reviews of any process function, data for rebuilding or repair and evidence for legal problems. Carefully and completely done calculations are easy to follow and leave no questions s to what was done and critically the basis of the calculations.

Documentation in calculations is critically important and properly done reduces errors in units. Most engineers will understand the need and prepare calculation pages carefully. The effort required is minimal and indicates true concern for proper calculations.

Finding or generating physical properties ties directly to the calculations documentation effort, these also require documentation. Many sources of physical properties are available and among that data is a lot of incorrect data. Selecting the proper data source can be tricky and frequently may require more than one source. The engineer needs to verify the data sources he / she is using.

REFERENCES

Perry's Chemical Engineers' Handbook, 6th Ed.

CRC Handbook of and Physics and Chemistry, 40thed.

"Clausius-Clapeyron Equation for Some Common Liquids" from the Wolfram Demonstrations Projecthttp://demonstrations.wolfram.com/ClausiusClapeyronEquationForSomeCommonLiquids/

Cetiner Engineering Corporation, "Physical Properties of Methanol"; http://cetiner.tripod.com/Properties.htm

Professional Publications "Chemical Engineering Reference Manual for the PE Exam"; 5th ed