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Curve fit equations for saturation vapor pressure of water.

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Cold Trap CFD Modeling for TEF KTI
[project 20.06002.01.091 (use to be 20.01402.661)]

1/29/03 STG

This notebook is intended to document the technical support provided for the effort on modeling the heat transfer and fluid flow phenomenon in the underground storage tunnels (drifts) for nuclear waste packages. This includes review and analysis of laboratory scale cold trap experiments and predictions of the actual field conditions at the actual storage facility.

The other team members for the overall effort are Randy Fedors (team leader), David Walter, and Frank Dodge.

My part of the task will involve standard engineering analysis and acting as a technical advisor to David Walter in his use of the FLOW-3D® CFD software package.

3/25/03 STG

Problem:

The CFD model of the cold trap phenomenon simulates dry air only. The CFD results are used to conduct a water vapor transport analysis to estimate the flow of water vapor from the hot end of the drift to the cold end. The analysis assumes that the air is saturated. The water vapor concentration is dictated by the vapor pressure of water at the local value of air temperature and some way of approximating the tabulated values of water saturation pressure is required. The temperature range of the air is approximately 20°C to 100°C

Required:

Determine a reasonably accurate correlation for the saturation vapor pressure of water in the specified temperature range.

Solution:

Investigate and compare the three correlations presented in Chapter 5 of ASHRAE Handbook of Fundamentals (1977):

Goff Formula (vapor pressure over liquid water for the temperature range of –50°C to 100°C):

$$\begin{aligned}\log_{10}(P_{v,sat}) = {} & 10.79586(1-\theta) + 5.82808\log_{10}(\theta) \\ & + 1.50474\times 10^{-4}\left(1-10^{-8.29692(1/\theta-1)}\right) \\ & + 4.2873\times 10^{-3}\left(10^{4.76955(1-\theta)}-1\right) \\ & - 2.2195983\end{aligned}$$

where

$$\theta = \frac{273.16}{T}$$

T = absolute temperature, Kelvin

$P_{v,sat}$ = water liquid - vapor saturation pressure, atmospheres

IMPORTANT NOTE:

The ASHRAE Fundamentals text had the coefficient of the Goff formula fourth term, 4.2873, listed as 0.42873. In conducting this review, it was discovered that the value, 4.2873, provided results that were more accurate than those given by the as-printed equation. I did not locate the original reference to verify the formula; rather, I assumed that the 'modified' equation listed here is the intended form

The citation for this equation is:

> Goff, J. A., "Saturation Pressure of Water on the new Kelvin Scale," ***Humidity and Moisture Measurement and Control in Science and Industry,*** Jwexler, A., and Wildhack, W. H., eds., Reinhold Publishing Corp., New York, 1965, p. 289. As cited in Chapter 5 of ***ASHRAE Handbook and Product Directory, 1977 Fundamentals***, Third Printing, American Society of Heating Refrigeration and Air Conditioning Engineers, Inc., New York, p. 5.12

Keenan, Keyes, Hill, and Moore Formula (vapor pressure over liquid water for the temperature range of 0°C to 374°C):

$$\ln\left(\frac{P_{v,sat}}{217.99}\right) = \frac{0.01}{T}(374.136-t)\left[-741.9242 + \sum_{i=1}^{7} F_i(0.65-0.01t)^i\right]$$

where

$F_1 = -29.72100$ $F_5 = +0.439993$

$F_2 = -11.55286$ $F_6 = +0.2520658$

$F_3 = -0.8685635$ $F_7 = +0.05218684$

$F_4 = +0.1094098$

$t = T - 273.15K = \text{degreed Celsius}$

$T = \text{absolute temperature, Kelvin}$

$P_{v,sat} = \text{water liquid - vapor saturation pressure, atmospheres}$

The citation for this equation is:

Keenan, J. H., Keyes, F. G., Hill, P. G., Moore, J. G., ***Steam Tables: Thermodynamic Properties of Water, Including Vapor, Liquid, and Solid Phases***, John Wiley and Sons, Inc, 1969. As cited in Chapter 5 of ***ASHRAE Handbook and Product Directory, 1977 Fundamentals***, Third Printing, American Society of Heating Refrigeration and Air Conditioning Engineers, Inc., New York, p. 5.12.

Keenan-Keyes Formula (vapor pressure over liquid water for the temperature range of 10°C to 150°C):

$$\log_{10}\left(\frac{P_{v,sat}}{218.167}\right) = \frac{\beta}{T}\left(\frac{a + b\beta + c\beta^3}{1 + d\beta}\right)$$

where

$$a = 3.2437814$$

$$b = 5.868276 \times 10^{-3}$$

$$c = 1.1702379 \times 10^{-8}$$

$$d = 2.1878462 \times 10^{-3}$$

$$\beta = 647.27 - T$$

$$T = \text{absolute temperature, Kelvin}$$

$$P_{v,sat} = \text{water liquid - vapor saturation pressure, atmospheres}$$

The citation for this equation is:

> Keenan, J. H., and Keyes, F. G., Hill, P. G., Moore, J. G., ***Thermodynamic Properties of Steam***, John Wiley and Sons, Inc, 1936, p. 14. As cited in Chapter 5 of ***ASHRAE Handbook and Product Directory, 1977 Fundamentals***, Third Printing, American Society of Heating Refrigeration and Air Conditioning Engineers, Inc., New York, p. 5.12.

These three equations were programmed into Excel (located in S. Green's desktop computer as C:\Projects\div20\Notebook\Water_Pvsat.xls)and compared to the tabulated values for the saturation pressure of water vapor in equilibrium with liquid water in the temperature range of 0.01°C to 200°C. The tabulated values are taken from

> Keenan, J. H., Keyes, F. G., Hill, P. G., Moore, J. G., ***Steam Tables***, John Wiley and Sons, Inc, New York, 1978. As cited in Appendix A of Van Wylen, G. J., and Sonntag, R. E., ***Fundamentals of Classical Thermodynamics,*** Third Edition, John Wiley and Sons, Inc, New York, 1985, p 613.

The tabulated values of the calculation results are shown on the following page and are compared graphically in the subsequent two figures.

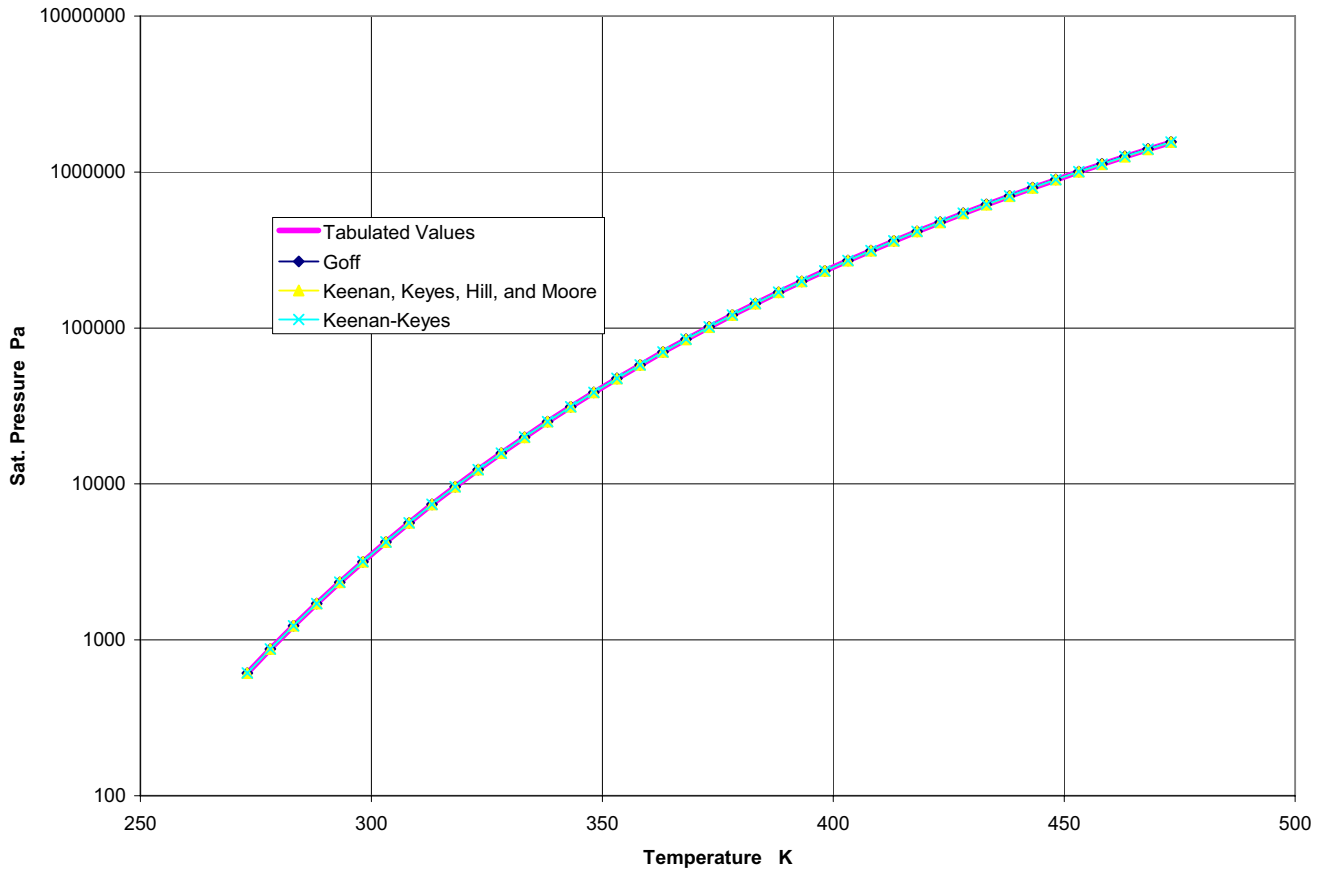
<u>Conclusion/Recommendation</u>

The saturation pressure graph shows that there are no serious deviations from the tabulated values in the recommended temperature range for each correlation. The correlation error graph, however, shows clearly that the Keenan, Keyes, Hill, and Moore correlation is superior to the other two. With current software packages, it is not much more difficult to code that correlation then the other two correlations.

It is recommended that the Keenan, Keyes, Hill, and Moore correlation be used for estimating the saturation pressure of water when the use of the tabulated experimental measurements is inconvenient.

Tabulated Values				Goff (-50°C to 100°C)				Keenan, Keyes, Hill, and Moore (0° to 374°C)				Keenan, Keyes (10° to 150°C)			
T	$P_{v,sat}$	T	$P_{v,sat}$	q	$P_{v,sat}$	$P_{v,sat}$	Error	t	$P_{v,sat}$	$P_{v,sat}$	Error	b	$P_{v,sat}$	$P_{v,sat}$	Error
C	kPa	K	Pa	1/K	atm	Pa	%	°C	atm	Pa	%	K	atm	Pa	%
0.01	0.6113	273.16	611.3	1	0.006037	611.863	0.092097	0.01	0.006033082	611.4529	0.025005	374.11	0.006052	613.411	0.345322
5	0.8721	278.15	872.1	0.98206	0.008612	872.848	0.085768	5	0.008606513	872.2701	0.01951	369.12	0.008629	874.5984	0.286483
10	1.2276	283.15	1227.6	0.964718	0.012122	1228.551	0.077465	10	0.012114683	1227.823	0.018171	364.12	0.012141	1230.491	0.235486
15	1.7051	288.15	1705.1	0.947978	0.016835	1706.24	0.066878	15	0.016826788	1705.395	0.017302	359.12	0.016856	1708.349	0.190519
20	2.339	293.15	2339	0.93181	0.023087	2339.88	0.037609	20	0.023078024	2338.958	-0.00181	354.12	0.023109	2342.132	0.133895
25	3.169	298.15	3169	0.916183	0.031284	3170.627	0.051348	25	0.031274455	3169.666	0.021017	349.12	0.031307	3173.004	0.12634
30	4.246	303.15	4246	0.901072	0.041913	4247.833	0.043167	30	0.041902799	4246.849	0.019987	344.12	0.041937	4250.332	0.102032
35	5.628	308.15	5628	0.886451	0.055551	5630.078	0.036928	35	0.055540631	5629.043	0.018532	339.12	0.055577	5632.736	0.084159
40	7.384	313.15	7384	0.872298	0.072879	7386.249	0.030456	40	0.072866911	7385.061	0.014374	334.12	0.072907	7389.165	0.06995
45	9.593	318.15	9593	0.858589	0.094688	9596.625	0.037785	45	0.094672707	9595.079	0.021671	329.12	0.094721	9599.996	0.072925
50	12.349	323.15	12349	0.845304	0.121894	12353.98	0.040319	50	0.121872015	12351.73	0.022096	324.12	0.121935	12358.14	0.074017
55	15.758	328.15	15758	0.832424	0.155547	15764.67	0.042329	55	0.155512524	15761.19	0.020271	319.12	0.155601	15770.15	0.077074
60	19.94	333.15	19940	0.819931	0.19684	19949.72	0.048729	60	0.196786237	19944.29	0.02149	314.12	0.196914	19957.27	0.086615
65	25.03	338.15	25030	0.807807	0.247122	25045.84	0.063286	65	0.247039798	25037.48	0.029898	309.12	0.247228	25056.54	0.106033
70	31.19	343.15	31190	0.796037	0.307908	31206.47	0.052813	70	0.307784428	31193.95	0.01267	304.12	0.308059	31221.74	0.101764
75	38.58	348.15	38580	0.784604	0.380885	38602.71	0.058853	75	0.380705361	38584.49	0.011634	299.12	0.381099	38624.37	0.115017
80	47.39	353.15	47390	0.773496	0.467925	47424.19	0.072153	80	0.467670679	47398.42	0.017774	294.12	0.468224	47454.54	0.136187
85	57.83	358.15	57830	0.762697	0.57109	57879.98	0.086431	85	0.570739467	57844.44	0.024978	289.12	0.571502	57921.74	0.158644
90	70.14	363.15	70140	0.752196	0.692642	70199.28	0.084518	90	0.692169212	70151.35	0.016181	284.12	0.693198	70255.64	0.164863
95	84.55	368.15	84550	0.74198	0.835048	84632.15	0.097164	95	0.834422398	84568.71	0.022129	279.12	0.835783	84706.65	0.185271
100	101.35	373.15	101350	0.732038	1.000988	101450.1	0.09881	100	1.00017224	101367.5	0.017224	274.12	1.001939	101546.6	0.19394
105	120.82	378.15	120820	0.722359	1.193358	120946.8	0.104987	105	1.192307562	120840.4	0.016861	269.12	1.194563	121069	0.20607
110	143.27	383.15	143270	0.712932	1.415278	143438.4	0.117526	110	1.413936779	143302.5	0.022679	264.12	1.416771	143589.7	0.223144
115	169.06	388.15	169060	0.703749	1.670092	169263.8	0.120573	115	1.66839102	169091.4	0.018591	259.12	1.6719	169447	0.228938

120	198.53	393.15	198530	0.694798	1.961378	198785.7	0.12878	120	1.959226397	198567.6	0.018937	254.12	1.963513	199002	0.237768
125	232.1	398.15	232100	0.686073	2.292945	232390	0.124937	125	2.290225478	232114.4	0.006184	249.12	2.295398	232638.6	0.232051
130	270.1	403.15	270100	0.677564	2.668839	270486.9	0.143233	130	2.665398004	270138.1	0.014101	244.12	2.671569	270763.5	0.245659
135	313	408.15	313000	0.669264	3.093347	313510.7	0.163163	135	3.088980926	313068.2	0.021795	239.12	3.096267	313806.6	0.257707
140	361.3	413.15	361300	0.661164	3.570995	361920.3	0.171686	140	3.565437834	361357.1	0.015811	234.12	3.573957	362220.6	0.254789
145	415.4	418.15	415400	0.653258	4.106554	416199.3	0.192411	145	4.099457859	415480.1	0.019272	229.12	4.109332	416480.8	0.260182
150	475.8	423.15	475800	0.645539	4.705044	476856.2	0.221989	150	4.695954148	475935	0.028363	224.12	4.707306	477085.5	0.270176
155	543.1	428.15	543100	0.638001	5.371732	544425	0.243973	155	5.360061992	543242.3	0.026198	219.12	5.373018	544555.3	0.267968
160	617.8	433.15	617800	0.630636	6.112137	619465.1	0.269522	160	6.097136702	617944.8	0.023439	214.12	6.111824	619433.3	0.264376
165	700.5	438.15	700500	0.623439	6.932036	702561.9	0.294343	165	6.912751325	700607.3	0.015324	209.12	6.929301	702284.6	0.254763
170	791.7	443.15	791700	0.616405	7.837464	794327	0.331815	170	7.812694287	791816.6	0.014724	204.12	7.831242	793696.4	0.252166
175	892	448.15	892000	0.609528	8.83472	895398.9	0.381042	175	8.802967022	892180.7	0.020259	199.12	8.823657	894277.7	0.255342
180	1002.1	453.15	1002100	0.602803	9.930374	1006443	0.433426	180	9.889781683	1002329	0.022889	194.12	9.912768	1004659	0.255367
185	1122.7	458.15	1122700	0.596224	11.13127	1128154	0.485798	185	11.07955896	1122913	0.018999	189.12	11.10501	1125493	0.248752
190	1254.4	463.15	1254400	0.589787	12.44453	1261253	0.546336	190	12.37892608	1254604	0.016275	184.12	12.40703	1257452	0.243343
195	1397.8	468.15	1397800	0.583488	13.87758	1406493	0.621878	195	13.794715	1398094	0.021059	179.12	13.82569	1401233	0.245632
200	1553.8	473.15	1553800	0.577322	15.43813	1564654	0.698561	200	15.33396087	1554097	0.01911	174.12	15.36805	1557552	0.241487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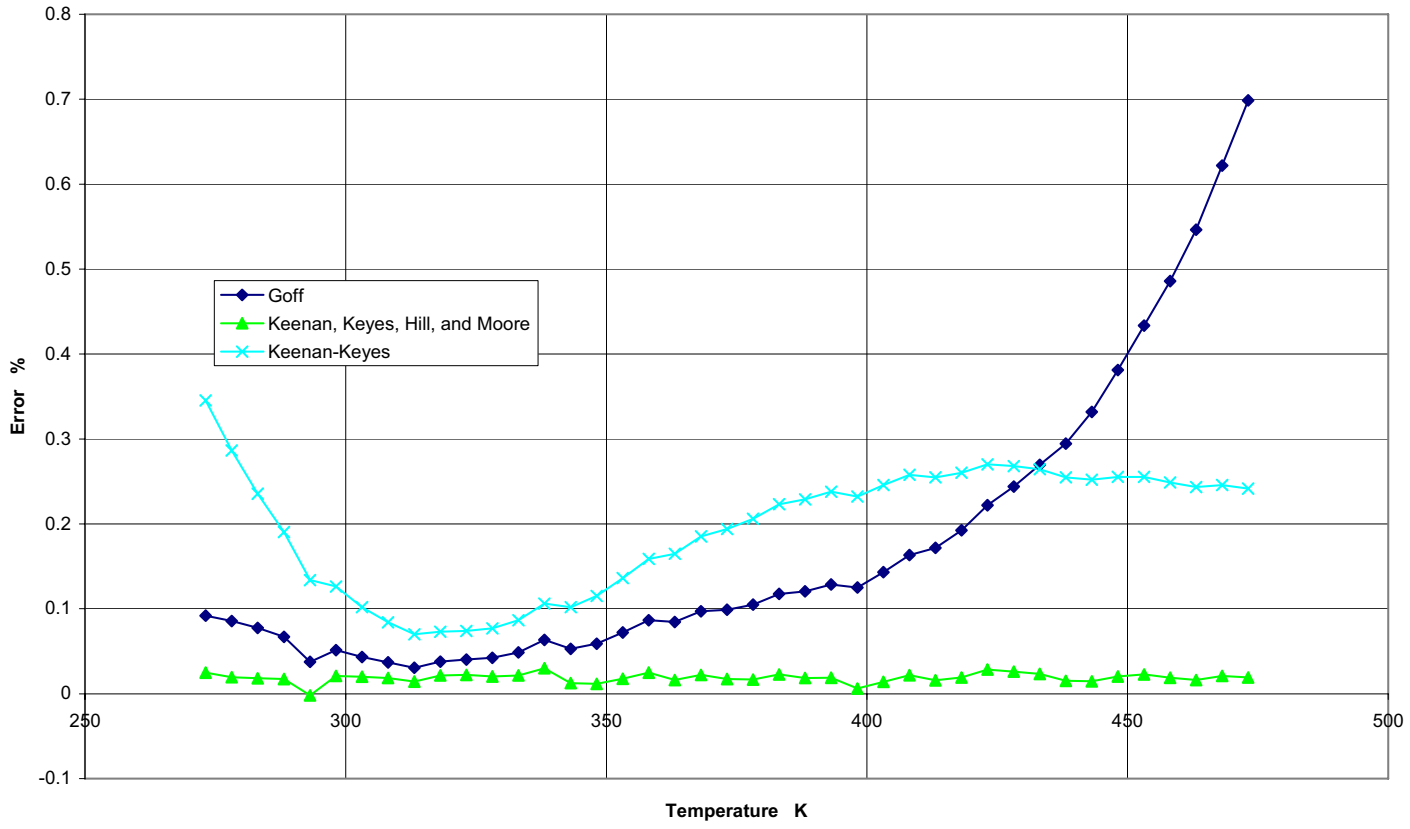
Tabulated Values
Goff
Keenan, Keyes, Hill, and Moore
Keenan-Keyes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