

Calculation of Superheated Steam Enthalpy and Density with the new 'Zpbe' equation for Pressures 1 - 140 Bar and Temperatures 100 – 700 Degr. Celsius.

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The newly discovered and modeled *Zpbe* equation as described in the previous post of 16 Nov 2020 [1] allows the compressibility factor Z to be calculated directly from a corresponding states relation written into a single cell of an (excel) spreadsheet for components with a *Zc* factor equal or close to 0.27.

In this post the *Zpbe* equation has been modified, in particular the temperature dependence, to allow application to Water which has a very different critical compressibility factor of *Zc* = 0.2294. With the help of this new *Zpbe-H2O* equation it is shown here that the Superheated Steam Enthalpy and Density can be straightforwardly calculated with high accuracy over a wide range of Superheated Steam pressures and temperatures.

Three equations will be presented below: 1) the Enthalpy of superheated Steam and 2) the Density of superheated Steam and 3) the *Zpbe-H2O* equation for superheated Steam.

Part I The three Equations

- 1) The enthalpy of superheated steam can be calculated from:

$$H_{steam}^{sup} = 1892 + 4.52 * Z_{pbe-H2O} * R / MW * T \quad \dots \dots \dots \text{(Eq. 1)}$$

The symbols have the following meaning: *Hsteam^{sup}* is the Enthalpy H of superheated steam in kJ /kg ; R is the Universal Gas Constant with value of 8.3145 kJ/kmol/oK ; MW is Mol. weight water is 18 ; T the absolute temperature in degrees Kelvin. The average percentage error compared with Grigull Steam Tables is 0.23 % over the following pressure and Temperature ranges: 1 < P < 140 Bar abs and 373 < T < 973 degr. Kelvin.

- 2) Density of superheated Steam:

$$D_{steam}^{sup} = P * 100 * MW / (Z_{pbe-H2O} * R * T) \quad \dots \dots \dots \text{(Eq.2)}$$

The symbols are: *Dsteam^{sup}* is the superheated steam density in kg per m3 ; P is the absolute pressure in Bar absolute ; other symbols as in equation (Eq.1). The average percentage error is 0.16% over the same range of conditions.

- 3) The compressibility factor Z for Superheated Steam:

$$Z_{pbe-H2O} = 1 - 0.3411 / Tr^{4.111} * Pr / (1 - 0.3411 / Tr^{4.111} * Pr) \quad \dots \dots \dots \text{(Eq.3)}$$

The symbol *Zpbe-H2O* stands for the compressibility factor of superheated steam ; the symbol Tr stands for the reduced Temperature equal to T / T_c in which the critical temperature is 647.14 degrees Kelvin ; and Pr stands for the reduced

pressure equal to P / P_c in which the critical pressure is 220.64 Bara abs. The average percentage error in calculated Z value is 0.16% !

Part II Some Calculation examples

To calculate the superheated steam enthalpy we begin first with Eq.3 to calculate the Z factor value for the pertinent conditions of practical interest.

(a) for a Steam Temperature of 375 oC and a Pressure of 60 Bara, with approx 100 degrees Celsius of superheat ; the reduced temperature $T_r = 1.001576$ and the reduced pressure $P_r = 0.271936$

$$Z_{pbe-h2o} = 1 - \frac{0.3411}{1.001576^4} \cdot 1.111 \cdot 0.271936 / (1 - \frac{0.3411}{1.001576^4} \cdot 1.111 \cdot 0.271936)$$

$$\Rightarrow Z_{pbe-h2o} = 0.8985 \text{ The Steam Table value is 0.9001.}$$

(b) Summary Table of some more examples

Examples Superheated Steam Operating Conditions & calculation Results						
	5	15	45	60	120	200
Oper. Pressure (Bar abs)	5	15	45	60	120	200
Reduced Pressure P_r	0.02266	0.06798	0.20400	0.27194	0.54387	0.90645
Oper. Temp. (Deg. Celsius)	225	300	400	400	500	450
Degrees Superheat (oC)	73	102	143	125	175	82
Abs. Temp. (Deg. Kelvin)	498.14	573.14	673.14	673.14	773.14	723.14
Reduced Temp. T_r	0.7698	0.8857	1.0402	1.0402	1.1947	1.1174
Calculation Results						
Calc. $Z_{pbe-h2o}$ (---)	0.9768	0.9603	0.9371	0.9144	0.9020	0.7564
Steam Table value Z (---)	0.9782	0.9620	0.9378	0.9152	0.9013	0.7611
Calc. $H_{steamup}$ (kJ/kg)	2908	3041	3209	3177	3348	3034
Steam Table value (kJ/kg)	2907	3036	3204	3177	3348	3060
Calc. $D_{steamup}$ (kg/m3)	2.226	5.905	15.457	21.12	37.29	79.22
Steam Table value (kg/m3)	2.223	5.894	15.446	21.10	37.13	78.73

Part III The Basis for the new $Z_{pbe-h2o}$ Equation for superheated Steam

In the previous post a new expression was found for the compressibility factor Z based on consideration and numerical data for the fugacity and the Z factor for compounds with a critical Z factor of 0.27. This equation was named the "Zpbe" equation. The form of this equation inspired a theoretical derivation for this equation (see post). This equation can be cast in the following form :

$$Z_{pbe} = 1 - K_{eq} * P_r / (1 - K_{eq} * P_r)$$

in which K_{eq} is the equilibrium constant. For compounds with a Z_c of 0.27 the equilibrium constant equals $K_{eq} = 0.333 / Tr^{3.905}$.

The question was how can this equation be applied to compounds with very different Z_c ! A compound like Water with its very low Z_c of 0.2294 ? Or for Lee-Kesler's " Simple Fluid with $Z_c=0.2901$ " ?

The answer was found in the realization of what the meaning of the equilibrium constant was, what it represented! In the developed model it stood for the ratio of fractions of molecules behaving like ideal gas and the fraction of molecules undergoing attraction forces; both fractions of gas molecules present in any real gas mixture below the critical temperature ($Tr < 1.0$).

Thinking of ideal gas we must think of gas particles only possessing kinetic energy! This means the mass and the velocity of the particle are influencing it's kinetic energy. Thus the mass hence the Molecular weight and the absolute temperature (no. of degr of freedom * kT) must influence the fraction of gas molecules behaving like ideal gas molecules in that real gas mixture at the given T and P ! And hence affect the equilibrium constant K_{eq} .

This reasoning lead to concluding that each compound has its own K_{eq} relation. The original equilibrium relation for compounds equal or close to $Z_c =0.27$ was found being :

$$K_{eq} = C_k / Tr^m \quad \text{with } C_k = 0.333 \text{ and exponent } m = 3.905$$

For Water, superheated Steam over a Temperature range of 100 – 700 oC and Pressures of 1 – 200 Bar abs I found:

$$K_{eq} = C_k / Tr^m \quad \text{with } C_k = 0.3411 \text{ and } m = 4.111$$

Similarly for Lee Kesler's "Simple Fluid $Z_c = 0.2901$ " I found

$$K_{eq} = C_k / Tr^m \quad \text{with } C_k = 0.320 \text{ and } m = 3.20$$

This latter relation I will come back to in a future post.

Ref. [1] Post of 16 Nov 2020 titled "Two simple yet accurate equations for calculating the fugacity coefficient phi and the gas compressibility factor Z.

<https://mychemengmusings.wordpress.com/2020/11/16/two-simple-yet-accurate-equations-for-calculating-the-fugacity-coefficient-phi-and-the-gas-compressibility-factor-z/>

Attached excel worksheet Superheated steam Table values plus calculations (2 pages)

End post.

Superheated STEAM Calculation of Superheated Steam Z values with the help of the new Zpbe-H2O equation

Comparison of calculated Zpbe-H2O values with Z-actual (derived from primary Steam Table values) Steam Tables from U.Grigull et al.

Tabulated data shown in bold

									Zpbe-h2o		Hsteamsuper		Dsteamsuper		
Superheated Steam			Degrees superheat	Saturation temp. oC	Superheated Steam		STEAM Density kg/m3	Z actual	Enthalpy Hv Table kJ/kg	m= 4.1110	stdev= 0.163	fct= 1.1300	stdev= 0.156	kJ/kg	stdev= 0.162
temp. oC	Temp. oK	T/Tc ---	oC	oC	Pressure Barabs	P/Pc ---				Ck = 0.34110	Error% 0.163	Uo= 1892	Error% 0.232	kg/m3	Error% 0.163
125	398.14	0.6152	25.2	99.8	1.0	0.00453	0.5503	0.989	2726	0.9885	0.04	2714	0.45	0.5506	0.04
150	423.14	0.6539	50.2	99.8	1.0	0.00453	0.5164	0.992	2776	0.9911	0.05	2768	0.30	0.5167	0.05
175	448.14	0.6925	75.2	99.8	1.0	0.00453	0.4867	0.993	2825	0.9929	0.05	2821	0.14	0.4869	0.05
200	473.14	0.7311	100.2	99.8	1.0	0.00453	0.4603	0.995	2874	0.9944	0.04	2874	0.01	0.4605	0.04
225	498.14	0.7698	125.2	99.8	1.0	0.00453	0.4368	0.996	2924	0.9954	0.03	2927	0.11	0.4370	0.03
250	523.14	0.8084	150.2	99.8	1.0	0.00453	0.4156	0.997	2973	0.9963	0.03	2980	0.24	0.4157	0.03
275	548.14	0.8470	175.2	99.8	1.0	0.00453	0.3964	0.997	3023	0.9969	0.02	3033	0.33	0.3965	0.02
300	573.14	0.8857	200.2	99.8	1.0	0.00453	0.3790	0.998	3073	0.9974	0.01	3086	0.41	0.3790	0.01
175	448.14	0.6925	23.0	152.0	5.0	0.02266	2.504	0.965	2800	0.9637	0.17	2794	0.22	2.5085	0.17
200	473.14	0.7311	48.0	152.0	5.0	0.02266	2.354	0.973	2854	0.9712	0.17	2851	0.09	2.3577	0.17
225	498.14	0.7698	73.0	152.0	5.0	0.02266	2.223	0.9782	2907	0.9768	0.15	2908	0.03	2.2264	0.15
250	523.14	0.8084	98.0	152.0	5.0	0.02266	2.108	0.982	2960	0.9811	0.12	2964	0.12	2.1107	0.12
275	548.14	0.8470	123.0	152.0	5.0	0.02266	2.006	0.985	3011	0.9845	0.09	3019	0.25	2.0076	0.09
300	573.14	0.8857	148.0	152.0	5.0	0.02266	1.914	0.988	3063	0.9871	0.06	3073	0.33	1.9149	0.06
325	598.14	0.9243	173.0	152.0	5.0	0.02266	1.830	0.990	3115	0.9892	0.05	3127	0.40	1.8310	0.05
200	473.14	0.7311	20.0	180.0	10	0.04532	4.857	0.943	2827	0.9407	0.24	2821	0.20	4.8683	0.24
225	498.14	0.7698	45.0	180.0	10	0.04532	4.555	0.955	2885	0.9525	0.25	2883	0.08	4.5665	0.25
250	523.14	0.8084	70.0	180.0	10	0.04532	4.298	0.964	2941	0.9615	0.21	2942	0.04	4.3076	0.21
275	548.14	0.8470	95.0	180.0	10	0.04532	4.075	0.970	2996	0.9684	0.16	3000	0.14	4.0817	0.16
300	573.14	0.8857	120.0	180.0	10	0.04532	3.877	0.975	3050	0.9739	0.13	3057	0.24	3.8819	0.13
325	598.14	0.9243	145.0	180.0	10	0.04532	3.700	0.979	3104	0.9782	0.09	3114	0.31	3.7033	0.09
350	623.14	0.9629	170.0	180.0	10	0.04532	3.540	0.982	3157	0.9816	0.06	3169	0.38	3.5422	0.06
225	498.14	0.7698	26.8	198.2	15.0	0.06798	7.018	0.930	2861	0.9270	0.29	2856	0.17	7.0379	0.29
250	523.14	0.8084	51.8	198.2	15.0	0.06798	6.582	0.944	2922	0.9411	0.29	2920	0.07	6.6013	0.29
275	548.14	0.8470	76.8	198.2	15.0	0.06798	6.214	0.954	2980	0.9519	0.23	2981	0.05	6.2289	0.24
300	573.14	0.8857	101.8	198.2	15.0	0.06798	5.894	0.9620	3036	0.9603	0.18	3041	0.17	5.9052	0.18
325	598.14	0.9243	126.8	198.2	15.0	0.06798	5.613	0.968	3092	0.9669	0.13	3099	0.24	5.6197	0.13
350	623.14	0.9629	151.8	198.2	15.0	0.06798	5.360	0.973	3147	0.9722	0.08	3157	0.31	5.3650	0.08
375	648.14	1.0015	176.8	198.2	15.0	0.06798	5.133	0.977	3201	0.9764	0.05	3213	0.38	5.1356	0.05
225	498.14	0.7698	12.8	212.2	20.0	0.09065	9.639	0.902	2834	0.9003	0.24	2828	0.20	9.6626	0.24
250	523.14	0.8084	37.8	212.2	20.0	0.09065	8.976	0.923	2901	0.9199	0.32	2897	0.15	9.0045	0.32
275	548.14	0.8470	62.8	212.2	20.0	0.09065	8.432	0.938	2963	0.9348	0.29	2962	0.04	8.4569	0.29
300	573.14	0.8857	87.8	212.2	20.0	0.09065	7.971	0.949	3022	0.9463	0.23	3024	0.08	7.9897	0.23
325	598.14	0.9243	112.8	212.2	20.0	0.09065	7.571	0.957	3080	0.9554	0.17	3085	0.16	7.5834	0.17
350	623.14	0.9629	137.8	212.2	20.0	0.09065	7.217	0.964	3136	0.9625	0.11	3144	0.26	7.2249	0.11
375	648.14	1.0015	162.8	212.2	20.0	0.09065	6.900	0.969	3192	0.9683	0.06	3202	0.32	6.9048	0.06
400	673.14	1.0402	187.8	212.2	20.0	0.09065	6.614	0.973	3247	0.9730	0.03	3259	0.38	6.6163	0.03
250	523.14	0.8084	26.3	223.7	25.0	0.11331	11.497	0.901	2879	0.8979	0.30	2873	0.22	11.5321	0.30
275	548.14	0.8470	51.3	223.7	25.0	0.11331	10.739	0.920	2945	0.9172	0.33	2942	0.11	10.7745	0.33
300	573.14	0.8857	76.3	223.7	25.0	0.11331	10.113	0.935	3007	0.9320	0.27	3007	0.01	10.1407	0.27
325	598.14	0.9243	101.3	223.7	25.0	0.11331	9.579	0.945	3067	0.9436	0.20	3070	0.11	9.5977	0.20
350	623.14	0.9629	126.3	223.7	25.0	0.11331	9.112	0.954	3125	0.9527	0.14	3132	0.21	9.1241	0.14
375	648.14	1.0015	151.3	223.7	25.0	0.11331	8.698	0.961	3182	0.9601	0.08	3191	0.29	8.7051	0.08
400	673.14	1.0402	176.3	223.7	25.0	0.11331	8.327	0.966	3239	0.9660	0.04	3250	0.33	8.3302	0.04
450	723.14	1.1174	226.3	223.7	25.0	0.11331	7.685	0.975	3350	0.9749	0.01	3364	0.42	7.6835	0.01
500	773.14	1.1947	276.3	223.7	25.0	0.11331	7.144	0.981	3462	0.9810	0.04	3476	0.39	7.1416	0.04
275	548.14	0.8470	17.9	257.1	45.0	0.20395	21.148	0.841	2862	0.8404	0.09	2854	0.29	21.167	0.09
300	573.14	0.8857	42.9	257.1	45.0	0.20395	19.481	0.873	2942	0.8706	0.31	2934	0.28	19.541	0.31
325	598.14	0.9243	67.9	257.1	45.0	0.20395	18.182	0.897	3013	0.8936	0.32	3008	0.17	18.242	0.33
350	623.14	0.9629	92.9	257.1	45.0	0.20395	17.141	0.913	3079	0.9116	0.14	3078	0.03	17.165	0.14
375	648.14	1.0015	117.9	257.1	45.0	0.20395	16.227	0.927	3143	0.9257	0.14	3145	0.06	16.250	0.14
400	673.14	1.0402	142.9	257.1	45.0	0.20395	15.446	0.9378	3204	0.9371	0.07	3209	0.16	15.457	0.07
450	723.14	1.1174	192.9	257.1	45.0	0.20395	14.138	0.954	3323	0.9539	0.02	3332	0.28	14.135	0.02
500	773.14	1.1947	242.9	257.1	45.0	0.20395	13.072	0.965	3439	0.9654	0.06	3450	0.33	13.064	0.06

Tabulated data shown in bold										STEAM		---- Zpbe-h2o ----		--- Hsteamsuper ---		--- Dsteamsuper ---	
Superheated Steam			Degrees superheat	Saturation temp.	Superheated Steam			STEAM Density kg/m3	Z actual	Enthalpy Hv Table kJ/kg	m=	stdev=	fct=	stdev=	kJ/kg	kg/m3	stdev=
temp. oC	Temp. oK	T/Tc ---	oC	oC	Pressure Barabs	P/Pc ---				4.1110	0.163	1.1300	0.156			0.162	
300	573.14	0.8857	24.8	275.2	60.0	0.27194	27.662	0.820	2883	0.8196	0.05	2873	0.35	27.674	0.05		
325	598.14	0.9243	49.8	275.2	60.0	0.27194	25.412	0.855	2967	0.8529	0.28	2957	0.33	25.482	0.28		
350	623.14	0.9629	74.8	275.2	60.0	0.27194	23.687	0.881	3042	0.8785	0.26	3035	0.23	23.748	0.26		
375	648.14	1.0015	99.8	275.2	60.0	0.27194	22.284	0.900	3111	0.8985	0.18	3108	0.10	22.324	0.18		
400	673.14	1.0402	124.8	275.2	60.0	0.27194	21.101	0.9152	3177	0.9144	0.10	3177	0.00	21.122	0.10		
450	723.14	1.1174	174.8	275.2	60.0	0.27194	19.180	0.937	3301	0.9376	0.03	3308	0.20	19.175	0.03		
500	773.14	1.1947	224.8	275.2	60.0	0.27194	17.653	0.953	3422	0.9533	0.08	3431	0.26	17.639	0.08		
325	598.14	0.9243	21.8	303.2	90.0	0.40790	42.996	0.758	2854	0.7619	0.48	2843	0.37	42.791	0.48		
350	623.14	0.9629	46.8	303.2	90.0	0.40790	38.776	0.807	2955	0.8059	0.14	2941	0.49	38.829	0.14		
375	648.14	1.0015	71.8	303.2	90.0	0.40790	35.760	0.841	3040	0.8396	0.21	3028	0.39	35.836	0.21		
400	673.14	1.0402	96.8	303.2	90.0	0.40790	33.410	0.867	3117	0.8658	0.15	3109	0.26	33.460	0.15		
450	723.14	1.1174	146.8	303.2	90.0	0.40790	29.855	0.9032	3256	0.9033	0.01	3256	0.00	29.852	0.01		
500	773.14	1.1947	196.8	303.2	90.0	0.40790	27.198	0.927	3386	0.9282	0.09	3390	0.13	27.173	0.09		
550	823.14	1.2720	246.8	303.2	90.0	0.40790	25.086	0.944	3510	0.9454	0.11	3517	0.19	25.058	0.11		
350	623.14	0.9629	24.9	325.1	120.0	0.54387	58.129	0.718	2846	0.7234	0.77	2833	0.45	57.683	0.77		
375	648.14	1.0015	49.9	325.1	120.0	0.54387	51.789	0.775	2958	0.7740	0.08	2939	0.63	51.829	0.08		
400	673.14	1.0402	74.9	325.1	120.0	0.54387	47.438	0.814	3050	0.8127	0.19	3034	0.52	47.530	0.19		
450	723.14	1.1174	124.9	325.1	120.0	0.54387	41.459	0.867	3208	0.8668	0.05	3201	0.23	41.479	0.05		
500	773.14	1.1947	174.9	325.1	120.0	0.54387	37.313	0.9013	3348	0.9020	0.08	3348	0.00	37.285	0.08		
550	823.14	1.2720	224.9	325.1	120.0	0.54387	34.152	0.925	3480	0.9259	0.11	3483	0.09	34.116	0.11		
360	633.14	0.9784	22.5	337.5	140.0	0.63452	69.430	0.6901	2808	0.6897	0.05	2804	0.15	69.462	0.05		
375	648.14	1.0015	37.5	337.5	140.0	0.63452	64.633	0.724	2893	0.7260	0.26	2874	0.64	64.464	0.26		
400	673.14	1.0402	62.5	337.5	140.0	0.63452	58.075	0.776	3001	0.7744	0.20	2980	0.69	58.192	0.20		
450	723.14	1.1174	112.5	337.5	140.0	0.63452	49.813	0.842	3174	0.8411	0.12	3162	0.38	49.872	0.12		
500	773.14	1.1947	162.5	337.5	140.0	0.63452	44.411	0.883	3322	0.8837	0.03	3319	0.10	44.397	0.03		
550	823.14	1.2720	212.5	337.5	140.0	0.63452	40.422	0.912	3459	0.9124	0.08	3460	0.03	40.388	0.08		
600	873.14	1.3492	262.5	337.5	140.0	0.63452	37.274	0.932	3590	0.9326	0.06	3592	0.06	37.254	0.06		
375	648.14	1.0015	26.3	348.7	160.0	0.72516	80.212	0.667	2818	0.6741	1.09	2804	0.49	79.345	1.08		
400	673.14	1.0402	51.3	348.7	160.0	0.72516	70.102	0.735	2946	0.7336	0.15	2923	0.78	70.205	0.15		
450	723.14	1.1174	101.3	348.7	160.0	0.72516	58.744	0.816	3138	0.8142	0.23	3121	0.53	58.881	0.23		
500	773.14	1.1947	151.3	348.7	160.0	0.72516	51.824	0.865	3295	0.8649	0.04	3288	0.21	51.846	0.04		
550	823.14	1.2720	201.3	348.7	160.0	0.72516	46.882	0.898	3438	0.8987	0.04	3436	0.04	46.865	0.04		
600	873.14	1.3492	251.3	348.7	160.0	0.72516	43.064	0.922	3572	0.9222	0.02	3573	0.03	43.055	0.02		
650	923.14	1.4265	301.3	348.7	160.0	0.72516	39.973	0.939	3703	0.9391	0.04	3702	0.03	39.990	0.04		
400	673.14	1.0402	36.1	363.9	190.0	0.86113	91.87	0.666	2852	0.6670	0.19	2829	0.79	91.692	0.19		
450	723.14	1.1174	86.1	363.9	190.0	0.86113	73.432	0.775	3081	0.7714	0.50	3057	0.79	73.802	0.50		
500	773.14	1.1947	136.1	363.9	190.0	0.86113	63.597	0.837	3253	0.8354	0.23	3240	0.39	63.742	0.23		
550	823.14	1.2720	186.1	363.9	190.0	0.86113	56.961	0.878	3405	0.8773	0.08	3400	0.15	57.005	0.08		
600	873.14	1.3492	236.1	363.9	190.0	0.86113	51.994	0.907	3545	0.9062	0.07	3544	0.03	52.028	0.07		
400	673.14	1.0402	31.5	368.5	200.0	0.90645	100.54	0.640	2816	0.6432	0.46	2796	0.71	100.086	0.46		
450	723.14	1.1174	81.5	368.5	200.0	0.90645	78.734	0.7611	3060	0.7564	0.62	3034	0.85	79.223	0.62		
500	773.14	1.1947	131.5	368.5	200.0	0.90645	67.709	0.828	3239	0.8252	0.32	3224	0.46	67.924	0.32		
550	823.14	1.2720	181.5	368.5	200.0	0.90645	60.427	0.871	3393	0.8700	0.14	3387	0.17	60.509	0.14		
600	873.14	1.3492	231.5	368.5	200.0	0.90645	55.039	0.902	3536	0.9008	0.10	3534	0.05	55.096	0.10		
650	923.14	1.4265	281.5	368.5	200.0	0.90645	50.795	0.924	3672	0.9227	0.16	3670	0.05	50.877	0.16		