Compressibility Factor Z for sub-critical pressures for Lee-Kesler's "Simple, Normal Fluids" Z-LK with a new set of compact equations for excel spreadsheets.

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This post presents a set of simple, compact equations to calculate the Compressibility factor Z based on Lee-Kesler's original publication stating: Z-LK = Z(0) + Omega * Z(1). The symbol Z(0) stands for the compressibility factor contribution of a "Simple Fluid with Zc = 0.2901" and omega is the "Acentric Factor" while Z(1) stands for the residual contribution to the Lee-Kesler compressibility factor Z-LK.

(1) The equation for Z(0).

The following equation allows the Z(0) to be directly calculated from the reduced temperature Tr , and reduced pressure Pr :

Z(0) = 1 – (0.329 / Tr^3.30 * Pr) / (1 - 0.329 / Tr^3.30 * Pr) …………….Eq. 1

This equation is valid for the following conditions: 0 < Pr < = 1 and 0.8 < Tr < 2.
The average absolute average percentage error compared to Lee-Kesler's Z(0) Table values is 0.30%. For details about the development of this equation see the earlier posts referenced in [Ref. 1] and [Ref. 2].

(2) The equations for Z(1).

The meaning of Z(1) is described by Lee-Kesler in [Ref.3] as " the deviation of the compressibility factor of the real fluid (characterized by omega) from Z(0)". Z(1) is a function of the reduced pressure and reduced temperature. Its values have been tabulated in the referenced publication. The following equations capture these values for the sub-critical reduced pressure range 0 < Pr < = 1.

Z(1) = A * Pr^2 + B * Pr

in which A and B or sole functions of reduced temperature Tr.
For the reduced temperature range of: 1 < Tr < 2

A = 0.3551 * Exp(-1.4313 * Tr^2.35)
B = 0.21078 – 0.20836 * Tr^-7 - 0.

and for the reduced temperature region of: 0.8 < T < = 1

A = - 0.8668 + 0.8611 * Tr^3.60
B = - 0.05 - 3.145 * Exp (- 5.1554 * Tr^4)

A graphical representation of Z(1) calculated with these five equations is given in Section (4) of this post.

(3) Examples of Application in an excel spreadsheet.

The above formulas can straightforwardly be used in the cells of a spreadsheet. No need for special excel calculation tools. The following Diagram shows a block of cells showing the inputs and the steps with the above equations to calculate for pure n-Butane the Lee-Kesler compressibility Factor "Z-LK" for a series of reduced pressure and temperature conditions. The results are compared to experimentally determined Z factor data based on [Ref.4].

Input				Z-LK = Z(0) + W * Z(1)				Z Factor Lee-Kesler	Exptl Data	
Compound	Omega W	Pr	Tr	A	B	Z(0)	Z(1)	Z-LK	Exptl. Z	Error% Z-LK
n-C4	0.1931	0.02634	0.7292	-0.59055	-0.78211	0.9748	-0.0210	0.9708	0.9741	0.34
	0.1931	0.02634	0.8568	-0.37315	-0.24544	0.9854	-0.0067	0.9841	0.9845	0.04
	0.1931	0.02634	0.9997	-0.00663	-0.06825	0.9912	-0.0018	0.9909	0.9911	0.02
	0.1931	0.13172	0.8468	-0.39358	-0.27201	0.9189	-0.0427	0.9107	0.9169	0.68
	0.1931	0.13172	1.0585	0.06917	-0.05037	0.9627	-0.0054	0.9617	0.9605	0.12
	0.1931	0.13172	1.2937	0.02582	0.05523	0.9811	0.0077	0.9826	0.9823	0.03
	0.1931	0.39515	0.9409	-0.17527	-0.10532	0.8110	-0.0690	0.7977	0.8067	1.12
	0.1931	0.39515	1.1761	0.04369	0.02264	0.9176	0.0158	0.9207	0.9209	0.03
	0.1931	0.52687	0.9997	-0.00663	-0.06825	0.7901	-0.0378	0.7828	0.7890	0.79
	0.1931	0.92202	1.0585	0.06917	-0.05037	0.6641	0.0124	0.6665	0.6701	0.54
sat. cond	0.1931	*0.52687*	*0.9115*	-0.24995	-0.13956	0.6922	-0.1429	*0.6646*	*0.6638*	0.12
	0.1931	*0.39515*	*0.8757*	-0.33281	-0.20170	0.7477	-0.1317	0.7223	*0.7298*	1.03
	0.1931	*0.13172*	*0.7609*	-0.54482	-0.60861	0.8805	-0.0896	0.8632	*0.8754*	1.40
	0.1931	*0.02634*	*0.6405*	-0.69361	-1.37072	0.9608	-0.0366	0.9538	*0.9592*	0.57
	0.1931	*0.7903*	*0.9664*	-0.10539	-0.08505	0.5895	-0.1330	0.5638	*0.5221*	7.98

The next Diagram shows calculated Z-LK values for pure Carbon Dioxide. Note here that for reduced pressure of 1.3555 i.e. slightly beyond the formal validity pressure range still reasonable predictions are made. (exptl Z values from [Ref.5])

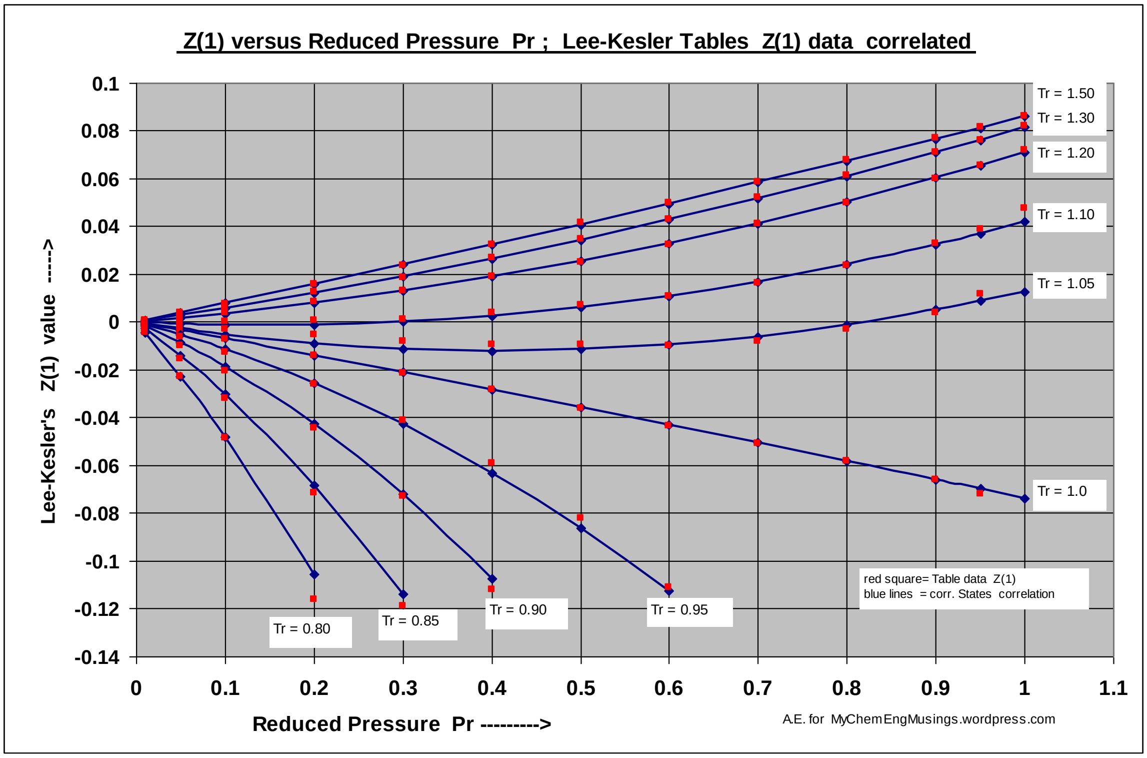
Compound	Omega W	Pr	Tr	A-(1)	B-(1)	Z(0)	Z(1)	Z-LK	Exptl. Z	Error% Z-LK
CO_2	0.2276	0.13555	1.0686	0.06666	-0.04137	0.9628	-0.0044	0.9618	0.9619	0.01
	0.2276	0.13555	1.3152	0.02328	0.05898	0.9816	0.0084	0.9835	0.9819	0.17
	0.2276	0.40665	0.9864	-0.04712	-0.07388	0.8372	-0.0378	0.8286	0.8352	0.79
	0.2276	0.40665	1.48	0.00974	0.07619	0.9619	0.0326	0.9693	0.9659	0.36
	0.2276	0.813306	1.1508	0.04849	0.01164	0.7976	0.0415	0.8071	0.8093	0.28
	0.2276	0.813306	1.644	0.00356	0.08317	0.9453	0.0700	0.9612	0.9591	0.22
	0.2276	0.948857	1.1508	0.04849	0.01164	0.7556	0.0547	0.7681	0.7737	0.73
	0.2276	1.3555	0.82202	-0.44156	-0.34876	-4.7339	-1.2841	-5.0262	?	?
	0.2276	1.3555	1.15083	0.04849	0.01165	0.6101	0.1049	0.6340	0.6610	4.09
	0.2276	1.3555	1.47964	0.00976	0.07617	0.8605	0.1212	0.8881	0.8936	0.61

Same but now for superheated steam:

Compound	Omega W	Pr	Tr	A-(1)	B-(1)	Z(0)	Z(1)	Z-LK	Exptl. Z	Error% Z-LK
H_2O	0.344	0.02266	0.7698	-0.53105	-0.56449	0.9820	-0.0131	0.9775	0.9782	0.07
super -	0.344	0.04532	0.8084	-0.46639	-0.39787	0.9690	-0.0190	0.9625	0.9635	0.11
heated	0.344	0.06798	0.8857	-0.31053	-0.18176	0.9655	-0.0138	0.9607	0.9620	0.13
Steam	0.344	0.11331	1.0015	0.08444	-0.11660	0.9615	-0.0121	0.9573	0.9619	0.48
	0.344	0.20395	1.0402	0.07387	-0.06854	0.9374	-0.0109	0.9336	0.9378	0.44
	0.344	0.27194	1.1174	0.05540	-0.00621	0.9339	0.0024	0.9347	0.9373	0.28
	0.344	0.4079	1.1174	0.05540	-0.00621	0.8974	0.0067	0.8997	0.9032	0.39
	0.344	0.63452	1.272	0.02859	0.05091	0.8958	0.0438	0.9109	0.9117	0.09
	0.344	0.86113	1.0402	0.07387	-0.06854	0.6689	-0.0042	0.6674	0.6657	0.26
	0.344	0.86113	1.1174	0.05540	-0.00621	0.7556	0.0357	0.7679	0.7753	0.96
	0.344	0.86113	1.1947	0.04038	0.02961	0.8130	0.0554	0.8321	0.8373	0.62
	0.344	0.86113	1.3492	0.01967	0.06398	0.8821	0.0697	0.9061	0.9068	0.08
	0.344	0.90645	1.1174	0.05540	-0.00621	0.7394	0.0399	0.7531	0.7611	1.05

(4) <u>Graphical representation of Z(1) with the help of the correlations in section(2</u>).

The following Excel Chart shows the Z(1) values calculated with the above correlations are shown as continuous blue lines. For comparison sake the Z(1) values from the Lee-Kesler Table for Z(1) are co-plotted and marked as red square points in the Chart.



(5) <u>References.</u>

[Ref.1] Post dated Nov 16, 2020 titled: "Two Simple yet Accurate Equations for Calculating the Fugacity Coefficient Phi and the Gas Compressibility Factor Z.

[Ref.2] Post dated May 26, 2021 titled: Lee-Kesler Simple Fluid (Zc 0.2901) Compressibility Z Factor for sub-critical pressures with the Z-pbe Equation in Excel Spreadsheets".

[Ref.3] Lee and Kesler 's publication titled " A Generalized Thermodynamic Correlation Based on Three Parameter Corresponding States" ; AIChE Journal (Vol. 21, no 3) , page 510, May, 1975.

[Ref.4] Buecker and Wagner, n-Butane Tables in: J. Chem. Ref. Data, Vol. 35, No 2, 2006, page 929 – 1018.

[Ref.5] Span and Wagner, CO2 Tables in: J. Chem. Ref. Data, Vol. 25, No 6, 1996, page 1509 – 1596.