A GENERALIZED CORRELATION FOR CRITICAL PRESSURE CALCULATION BASED ON AN INNOVATIVE IDEAL CRITICAL PRESSURE PARAMETER

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ABSTRACT

The availability of accurate thermophysical properties of fluids is essential in chemical process industries design and operations. While traditional hydrocarbon processing continue to be important, new emerging technologies involving advanced fuels and high-value chemicals will dramatically change the fluids-based industries. In the last years the availability of virtual tools for fluids properties calculation has rapidly accelerate but, at the same time, the dependence of these tools on robust thermodynamic models validated on accurate experimental data has been, often, unrecognized. Within this contest, the evaluation of critical parameters is of great interest as they are widely involved in predictive properties models for both pure substances and multi-components mixtures.

This work investigates the potentiality of a new generalized correlation in calculating the critical pressure of compounds belonging to aliphatic hydrocarbons comprehensive of ubranched, branched, alkenes and alkines. This idea has emerged considering that, for a total of 90 aliphatic compounds, the critical pressure is available as recommended data [1]. If these data are correlated Vs. an innovative parameter introduced in this work and identified as *ideal critical pressure,* the resulting function can be simply expressed through a linear relationship reaching a coefficient of determination (R^2) equal to 0.9958.

The main advantage of the proposed method is that the critical pressure can be directly calculated by knowing only the critical temperature and the critical volume of the compounds. From this point of view it significantly differs from most of the available models usually based on group contributions method requiring a relevant number of parameters and, in some cases, complex formulations. Reference is made to the methods proposed by Ambrose [2], Joback [3], Somayjulu [4], Jalowka-Daubert [5], Constantinou-Gani [6] and Marrero-Pardillo [7]. Within this paper, these models are synthetically presented and their performances compared with the proposed correlation, whose quality, expressed in terms of Absolute Average Deviation (AAD%) reaches, for unbranched alkanes, the value of 2,31%, for alkenes and alkynes 1,84%. These results are significant better if compared with those achieved by the cited models for the same investigated hydrocarbons families.

Further, the proposed correlation has been tested in predicting the critical pressure of other families of fluids for a total amount of 170 compounds as: cyclic hydrocarbons, halogenated alkanes, hydrofluoroethers and others hydrocarbons not included inside the recommended initial list. The previous indicated performances are confirmed for these families of fluids too. If, for some compounds, the required input critical parameters are unknown, they can be estimated by using some formulations defined by the Authors of the models here cited for comparison. As case test, this predictive methodology has also been implemented in this study for several compounds, confirming the declared performances. For the simplicity of the computational procedure and the limited amount of the input parameters, the proposed approach can be easily implemented by working well also in a complete predictive mode.

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