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Tuning Cubic Equations of State for Supercritical Water Applications

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Abstract : Cubic equations of state (EoS), popular due to their simple mathematical form, ease of use, semi-theoretical nature and, reasonable accuracy are normally fitted to vapor-liquid equilibrium P-v-T data. As a result, They often show poor accuracy in the region near and above the critical point. In this study, the performance of the renowned Peng-Robinson (PR) and Patel-Teja (PT) EoS's around the critical area has been examined against the P-v-T data of water. Both of them display large deviations at critical point. For instance, PR-EoS exhibits discrepancies as high as 47% for the specific volume, 28% for the enthalpy departure and 43% for the entropy departure at critical point. It is shown that incorporating P-v-T data of the supercritical region into the retuning of a cubic EoS can improve its performance above the critical point dramatically. Adopting a retuned acentric factor of 0.5491 instead of its genuine value of 0.344 for water in PR-EoS and a new F of 0.8854 instead of its original value of 0.6898 for water in PT-EoS reduces the discrepancies to about one third or less.

Keywords : equation of state, EoS, supercritical water, SCW
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