

# **Novel Computational Algorithm on Intelligent Application of Molecular Structure Information, PVT Data and Equations of State on Determination of Thermo-Physical Properties of Polymeric Systems**

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For the successful and reliable modeling, simulation, design and control of processes involve the polymeric materials, such as membrane fabrication from polymeric solutions, the thermo-physical properties such as PVT data, critical properties, solubility parameters, etc. are required. A number of advantageous outcomes were obtained through our investigations on determination of thermo-physical properties of polymeric systems as listed below, which were made possible by the introduction and application of a simple novel computational algorithm on intelligent coupling of molecular structure information, PVT data and equations of state.

# 1 - Modified group contribution method for accurate estimation of thermo-physical properties

# 2 - Molecular structure based method to define the PVT relationships in the form of Tait equation

# 3 - Algorithm to adapt any equation of state (EOS) for thermo-physical properties and phase calculation of polymeric systems, in particular cubic EOS

The research methodology involves these steps;

(i) The available literatures were reviewed to retrieve information on PVT data of polymeric systems in the form of tabulated data point, empirical models, theoretical models etc.

(ii) A well-established group contribution method was modified by introducing a chemical structure descriptors based function as results in # 1.

(iii) The data of steps (i) and (ii) were used to tailor a generic cubic equation of state as results in #3.

(iv) since the equations of state represent PVT data, by implementation of modified group contribution method (#2), the equations of states available in literatures were used to develop Tait model for (1) all systems of step (i) to check the EOS consistency and then (2) for other interested systems as results in #2.

The proposed algorithm and all aforementioned obtained results have been presented and discussed in details.