Prediction of Phase Transition Temperature and Enthalpy of Normal Alkanes together with Heat Capacity from Ordered Solid to Liquid Phase

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New models have been developed to predict the thermophysical properties related to the phase transition of normal alkanes which are the most encountered components in the petroleum industry. The calculations include temperature and enthalpy of solid-liquid (fusion) and order-disorder solid phase transition of pure normal alkanes in addition to the temperature dependency of heat capacity in aforementioned phases as a function of carbon number. For the fusion temperature, 67 experimental data points in the carbon range of 1 to 390 have been used to develop two correlations while 41 experimental data in the carbon range of 1 to 60 have been used to correlate enthalpy of solid-liquid phase transition. Also, 26 experimental data in the carbon range of 9 to 44 have been used to correlate the temperature and another 23 data have been used to obtain the correlation for enthalpy of order-disorder solid phase transition as well as a new model for the estimation of total phase change enthalpy by using the experimental data of fusion and order-disorder solid phase transition. Due to the difference of heat capacity in the liquid, disorder solid and order solid, three heat capacity models have been presented based on the group contribution approach for a wide range of carbon number as a function of temperature according to the available experimental data. Average absolute deviation percent (AAD %) of the new models has been obtained 0.66, 3.47, 0.35, 4.09, 7.52, 0.54, 4.65 and 6.89 for fusion temperature, fusion enthalpy, order-disorder solid phase transition temperature, order-disorder solid phase transition enthalpy, total phase change enthalpy, heat capacity in liquid, disorder and order solid phase, respectively, by more than 1300 experimental data points. The results demonstrate that these new approaches are in more agreement with experimental data in comparison with the other methods presented in the literature.