Prediction Models for the Flash Point of Pure Components

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ABSTRACT

The flash point for a liquid is defined as the lowest temperature at which its vapor form a spontaneously ignitable mixture when brought in contact with air. In principle, the vapors are expected to burn at this point but only briefly. The relevance of having a good estimation of the flash point temperature ($T_f$) is because it is one of the main properties used to characterize fire and explosion hazard of liquids. The flash point is not considered a fundamental property since it is defined by the specific experimental system and procedure used (Crowl and Louvar, 2002). The most common experimental methods used to determine the flash point are the open and the closed cup. The open-cup apparatus produces flash point values a few degrees higher than closed-cup system. There is no theoretical method developed to estimate $T_f$ but several correlations have been proposed. The current models relate the flash point temperature with one or a combination of variables such as the boiling temperature ($T_b$), vapour pressure, standard heat of formation and the standard heat of combustion, some of which apply different parameter values for different chemical groups (Satyanarayana and Rao, 1992; Gharagheizi, 2009). In this study, it was observed for 694 pure compounds that the relation $T_f / T_b$ remains around a constant value. Thus, a thumb rule indicates that the $T_f$ is 0.76 times $T_b$ within an average error of 0.36% and an absolute average error of 4.4%. The dispersion around this value is considered here a function of both physical and chemical properties. Considering that the liquid molecules should be evaporated to burn, the vaporization change of enthalpy ($\Delta H_v$) is included in our model. In addition, the heat of combustion ($\Delta H_c$) is included to incorporate a chemical behavior in the model. Thus, the thumb rule is expanded to include the dimensionless group ($\Delta H_v/\Delta H_c$ ). Given the lack of experimental data, the number of components used to produce the new correlation was substantially reduced to 45 species, and the average error was reduced to 0.15 % whereas the absolute average error to 2.71%. The model has been also validated by using the ASPEN package to estimate the unknown data, mainly ($\Delta H_c$), for some of the compounds.

References

