

## Estimation of Paraffin Pour Points

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Wax precipitation is an undesirable problem in the oil industry because it causes plugging of pipelines, reservoirs, and process equipment. This precipitation and deposition of paraffin waxes from crude oils is commonly observed in production, transportation, and processing operations. To anticipate and mitigate this problem, it is important to estimate the pour point, which is the temperature at which the liquid-solid mixture loses its flow characteristics. To enable process engineers to easily estimate the pour point and related properties, a thermodynamic model has been developed in Aspen Plus. The model has been compared to various sources of literature data to evaluate its reliability and accuracy.

Aspen Plus has a framework in which pure solids can precipitate from a liquid. However, in the case of paraffins the solids form a mixture. Aspen Plus, in principle, has the framework in which solid mixtures can precipitate, however this system is error prone and hence could not be reliably used. An alternate framework has been created in which each paraffin that could precipitate (C<sub>12</sub> or *n*-dodecane to C<sub>34</sub> or *n*-tetratriacontane in the present component slate) is treated via a Chemistry model that describes the equilibrium between the solid and liquid forms using the standard thermodynamic framework in terms of the triple-point temperature, the enthalpy of fusion, and the difference between the solid and liquid heat capacities.

The solid-liquid equilibrium calculation has been simulated via a pseudo liquid-liquid equilibrium calculation. The NRTL activity-coefficient model has been used and the activity coefficients between the solid and liquid components have been set to a very large value (10<sup>6</sup> or 1 million appears to be sufficiently large) so that the mutual solubility is effectively zero. Next the activity coefficients among the liquid components and the solid components need to be modeled. In contrast to the conclusions of most researchers, we have found that the liquid phase can be modeled as ideal, i.e., following Raoult's law. Various models for the solid phase were tested, and the model that worked adequately for the solid is one where the temperature-independent infinite-dilution activity coefficient for a particular solid-solid pair is given by a simple function in terms of the difference in carbon numbers of the two components.

Comparison with literature data shows that this simple model provides an accurate prediction for a wide range of data.