



## Full Length Article

# Prediction of thermal conductivity for characterized oils and their fractions using an expanded fluid based model

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## ABSTRACT

A methodology is proposed to predict the thermal conductivity of crude oils (mainly heavy oils) and their fractions based on a distillation assay, asphaltene content, molecular weight, and specific gravity of the fluid. The oils are characterized into a set of pseudo-components and their thermal conductivity is calculated using the Expanded Fluid (EF) thermal conductivity model. The inputs of this model are: the density of the fluid, the pressure, the dilute gas thermal conductivity, and, four parameters that are required for each pseudo-component,  $\rho_s^\circ$ ,  $\lambda_s^\circ$ ,  $c_{2\lambda}$ , and  $c_{3\lambda}$ . The dilute gas thermal conductivity and the parameter  $\rho_s^\circ$  are calculated from existing correlations. New correlations are proposed for the remaining model parameters and for the binary interaction parameters used in the model mixing rules. The proposed approach was developed and tested on thermal conductivity and density data from the literature for pure hydrocarbons, pure hydrocarbon binaries, bitumen/solvent pseudo-binaries, crude oils, and distillation cuts. In addition, thermal conductivity and density data for pseudo-binaries of C5-asphaltene and toluene were collected in this study at temperatures from 20 to 40 °C and pressures up to 10 MPa. The EF thermal conductivity model with correlated fluid-specific parameters predicted the thermal conductivity of 7 crude oils from disparate geographical locations within 3% of the experimental data. Deviations were reduced to within 1% of experimental data by either tuning  $\rho_s^\circ$  to a viscosity data point or tuning  $\lambda_s^\circ$  to a thermal conductivity data point.

## 1. Introduction

Reliable thermal conductivity values for crude oils are required over a wide range of temperatures, pressures, and compositions for the design of heat transfer and non-isothermal mass transfer operations in petroleum processes such as refineries [1]. Thermal conductivity is also an input in the modeling of thermal *in situ* recovery processes [2,3]. The fluids in these operations may be blends of oils, fractions of oils, or phases separated from an oil. Since it is impractical and sometimes impossible to measure thermal conductivity under all conditions, a method is required to accurately predict the thermal conductivity of each fluid as a function of its composition at any temperature and pressure.

Crude oils contain hundreds of thousands of components [4] and their composition and property distributions are typically represented with a set of components and pseudo-components. For phase behavior modeling in process simulation, the components and pseudo-components are usually defined based on boiling point intervals [5]. The mass fraction of each boiling point interval (*i.e.* pseudo-component) is

assigned based on a distillation assay usually obtained from true boiling point distillation [6] or simulated distillation [7]. Since not all of the oil is distillable (for example, less than 50 wt% of a heavy oil is distillable), the distillable fraction data must be extrapolated to define the heavy fractions and complete the oil characterization [8]. Once the pseudo-components are defined, the specific gravity, molecular weight, critical properties, and acentric factor of each pseudo-component are determined from correlations. Finally, the physical properties of the crude oil are calculated by combining the properties of the pseudo-components. This approach can be extended to thermal conductivity modeling.

Although there are several models and correlations to calculate the thermal conductivity of fluids, they are only applicable to pure hydrocarbons and to mixtures of well-defined components [9]. Only a few models are suitable for mixtures of ill-defined components such as petroleum distillation cuts and pseudo-components. Those models can be divided into two groups: liquid phase models and fluid phase models. The two fluid phase models considered here are the Corresponding States and Expanded Fluid approaches. The models in the first

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group are only applicable to liquids far from the critical point while those in the second group are applicable across the fluid phase diagram including the gas, liquid, and supercritical regions. Both liquid phase models and the two fluid phase models are briefly reviewed below.

**Liquid Phase Models:** The models in this group are empirical correlations that capture how the thermal conductivity of a liquid changes with temperature at atmospheric pressure and temperatures far below its critical temperature. For uncharacterized petroleum fractions, the API Technical Databook [10] recommends a linear correlation between thermal conductivity and the absolute temperature with specified values for the slope and intercept. For characterized fractions, the intercept and the slope are calculated as a function of the normal boiling point. Bland and Davidson [11] proposed another linear correlation for distillation cuts where the intercept and the slope are function of the specific gravity. They presented a chart to predict the thermal conductivity of petroleum fluids as a function of temperature and API gravity. Aboul-Seoud and Moharam [1] proposed a correlation for the thermal conductivity of distillation cuts based on the linear trend observed between thermal conductivity and the square root of the ratio specific gravity to absolute temperature. Teja and Tardieu [12] proposed an alternative approach where the thermal conductivity of a distillation cut at different temperatures is calculated as a function of its effective carbon number (ECN). The ECN of a substance is calculated from its thermal conductivity at a reduced temperature of 0.6. In general, these correlations predict the thermal conductivity of petroleum distillation cuts with normal boiling points below 550 °C with an average deviation within 6% and a maximum deviation within 25% of the experimental data.

**Corresponding States (CS) Fluid Phase Model:** This model calculates the thermal conductivity of a fluid as the sum of the thermal conductivity due to translational movement of molecules and the thermal conductivity due to internal degrees of freedom. Only the translational contribution follows the CS principle and is calculated from the CS model. The contribution due to internal degrees of freedom is calculated from expressions derived from the kinetic theory of gases [13]. The CS model relates the translational thermal conductivity of a fluid to the reduced translational thermal conductivity of a reference fluid at the same reduced temperature and density [13]. Shape factors have been included into the model in order to correct the non-correspondence of most fluids to the reference fluid (methane).

Christensen and Fredenslund [14] proposed an alternative CS model with reduced pressure as one of the coordinates instead of reduced density. Methane was used as reference fluid and a rotational coupling coefficient was proposed instead of shape factors. The authors also introduced a semi-empirical correlation for the estimation of the thermal conductivity due to internal degrees of freedom. Pedersen and Fredenslund [15] updated the original expression for the calculation of the rotational coupling coefficient by tuning it to a larger pure hydrocarbon and distillation cut dataset. This updated CS model version predicted thermal conductivity of 25 distillation cuts within 20% of the measured values.

Baltatu et al. [16] introduced a modification to the original Hanley CS model in the form of a density dependent correction factor. This version of the model uses propane as the reference fluid and also includes a shape factor that accounts for the relative aromatic and naphthenic contents of petroleum fractions. This version of the CS predicted the thermal conductivity of over 25 distillation cuts and coal derived liquids with an average absolute deviation of 7%.

All versions of the CS model are computationally intensive requiring iterative algorithms for the calculation of the reference fluid properties and model parameters. In addition, the application of the CS model to heavy petroleum fluids can be challenging because these fluids correspond to methane at temperatures below its freezing point.

**Expanded Fluid (EF) Model:** This model [17] is based on the observation that as a fluid expands, from the liquid-solid or liquid-glass phase transition to the dilute gas state, its thermal conductivity

decreases monotonically (except for the critical enhancement near the critical point). The inputs of the EF thermal conductivity model are the density of the fluid, the pressure, the dilute gas thermal conductivity, and four fluid-specific parameters:  $\rho_s^\circ$ ,  $\lambda_s^\circ$ ,  $c_{2\lambda}$  and  $c_{3\lambda}$ . The dilute gas thermal conductivity is calculated as a function of temperature using the Yaws [18] correlation. The value of the parameter  $\rho_s^\circ$  is calculated from viscosity data, with values of  $\rho_s^\circ$  having been reported for over 150 pure hydrocarbons [19–22]. The parameter  $\rho_s^\circ$  for distillation cuts and pseudo-components is predicted as a function of boiling point and specific gravity using the method proposed by Ramos-Pallares et al. [21]. The values of parameters  $\lambda_s^\circ$ ,  $c_{2\lambda}$  and  $c_{3\lambda}$  are determined by fitting the model to thermal conductivity data, and these values have been reported for over 50 pure hydrocarbons [17]. Compared to the CS model, the EF model converges rapidly because it does not require iterative calculations. It is also easily applied to heavy petroleum fluids. However, the EF thermal conductivity model has not been yet extended to distillation cuts and petroleum pseudo-components.

The objective of this study is to extend the EF thermal conductivity model to predict the thermal conductivity of petroleum fractions and characterized oils. The oils are to be characterized into pseudo-components based on a distillation assay using the same characterization methodology used to predict the viscosity of heavy oils with the EF viscosity model [21]. A framework is proposed for the extended model including correlations for the pseudo-component thermal conductivity model parameters and for the binary interaction parameters used in the model mixing rules. The proposed oil characterization and modeling methodology is developed and tested based on measured thermal conductivities of pure hydrocarbons, pure hydrocarbon binaries, bitumen/solvent pseudo-binaries, crude oils, and distillation cuts obtained from the literature. The dataset is supplemented with thermal conductivity and density data for pseudo-binaries of C5- asphaltene and toluene collected in this study at temperatures from 20 to 40 °C and pressures up to 10 MPa. A simple tuning procedure is proposed for cases where at least one viscosity and/or thermal conductivity measurement is available. Note, the proposed model does not apply to fluids containing solid phases, such as waxes and hydrates.

## 2. Experimental methods

Most of the data required to develop the model were reported previously [17] or taken from the literature. However, the density and thermal conductivity of solutions of C5-asphaltenes and toluene were required to test the model mixing rules when applied to asphaltenes. These data were not available and were collected as part of this study.

### 2.1. Materials

The asphaltenes were precipitated from a dead bitumen using a 40:1 ratio (mL/g) of *n*-pentane/bitumen following the procedure described by Ramos-Pallares et al. [21]. The asphaltenes obtained from this procedure are termed “C5-asphaltenes”. The bitumen is labeled as WC-B-A3(1) where WC = Western Canada, B = bitumen, A3 identifies a reservoir, and (1) is the sample number. The specific gravity, molecular weight, and C5-asphaltene content of the WC-B-A3(1) bitumen are 1.010, 550 g/mol, and 18 wt%, respectively [17]. Toluene (purity of 99.5%) was obtained from VWR.

### 2.2. Density measurements

Densities were measured in an oscillating U-tube Anton Paar DMA 4500 M density meter at atmospheric pressure. The temperature of the sample cell was controlled to within  $\pm 0.01$  °C of the measurement value by a Peltier mechanism enabling measurements from 0 °C to 90 °C. The samples were injected directly into the apparatus and their density was measured once thermal equilibrium was reached at a set temperature. The instrument was calibrated using reverse-osmosis

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