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A computational intelligence scheme for prediction of interfacial tension between pure hydrocarbons and water

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ABSTRACT

Interfacial tension plays a major role in many disciplines of science and engineering. Complex nature of this property has restricted most of the previous theoretical studies on thermophysical properties to bulk properties measured far from the interface. Considering the drawbacks and deficiencies of preexisting models, there is yet a huge interest in accurate determination of this property using a rather simple and more comprehensive modeling approach. In recent years, inductive machine learning algorithms have widely been applied in solving a variety of engineering problems. This study introduces least-square support vector machines (LS-SVM) approach as a viable and powerful tool for predicting the interfacial tension between pure hydrocarbon and water. Comparing the model to experimental data, an excellent agreement was observed yielding the overall squared correlation coefficient (R^2) of 0.993. Proposed model was also found to outperform when compared to some previously presented multiple regression models. An outlier detection method was also introduced to determine the model applicability domain and diagnose the outliers in the gathered dataset. Results of this study indicate that the model can be applied in systems over temperature ranges of 454.40–890 °R and pressure ranges of 0.1–300 MPa.

1. Introduction

Thermophysical properties of fluids are very important for engineering and industrial purposes. As a crucially important thermo-physical property, interfacial tension plays a vital role in describing the interface characteristics. Interfacial tension and its behavior are more complex than other thermophysical properties because it deals with surface and bulk characteristics of the system whereas other thermophysical properties only deal with bulk characteristics of the system (Dandekar, 1994).

The complexity and intricacy of the underlying molecular mechanisms have restricted most of the investigations to bulk system properties and traditionally not much attention has been paid to quantification and modeling of interfacial tension in comparison to other thermophysical properties.

When two immiscible or partially miscible fluids come into contact, lighter phase lays over heavier phase due to buoyancy

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Nomenclature

A^η	acceptance probability function
AARD	average absolute relative deviations (%)
b	bias term
C	positive constant
CSA	coupled simulated annealing
e	error variable
$g(x)$	mapping function
H	hat matrix
IFT	interfacial tension
J	cost function
$K(x,x_i)$	Kernel function
L	Lagrangian multipliers
LSSVM	least-squares supported vector machine
m	number of employed data
MSE	mean squared error
NO	number of training objects
n	total number of model parameters
R	residual
R^2	coefficient of determination
RMSE	root mean square errors
SA	simulated annealing
t	transpose operator
$T_{^\circ R}$	temperature in Rankin
$T_{c,h}$	critical temperature of hydrocarbon
$T_k{}^a$	acceptance temperature
w	a nonlinear function
x	inputs
X	a two dimensional matrix ($m \times n$)
y	outputs
β	Lagrangian multiplier
ρ_w	water density
ρ_h	hydrocarbon density
γ_{hw}	interfacial tension between hydrocarbon and water
Ψ	coupling term
σ^2	squared bandwidth
μ	regularization constant

effect. In this case, a thin layer with different properties than bulks of the fluids, separates the two phases.

This layer is referred to as the interface. In the bulk of each phase, a molecule is impacted by the same intermolecular interactions from all sides because of molecular similarity, so that the resultant of the forces acting on each molecule tends to zero. On the other side, each molecule on the interface experiences different intermolecular interactions from different sides because of different phases on each side of the interface having different chemical nature or molecular density which result in different intermolecular interactions (Aranda-Bravo et al., 2008).

As a result, overall quantity of interactive forces acting on each of interfacial molecules will be non-zero (Ling and He, 2012). The imbalance in the applied forces results in the attraction of the molecules toward the phase exercising stronger interactions.

This phenomenon is generally known as interfacial tension. In other word, interfacial tension could be thought of as a quantitative index indicating the molecular behavior at the interface (Dandekar, 1994). From another point of view, interfacial tension is defined as the change in Gibbs free energy per unit change of interfacial area at defined temperature, pressure and chemical composition and is expressed as below (Demond and Lindner, 1993):

$$\left(\frac{\partial G}{\partial A}\right)_{T,P,n} = \gamma \tag{1}$$

In Eq. (1), G is Gibbs free energy, A is interfacial area, T is temperature, P is pressure and n is chemical composition. IFT is usually expressed as the force per unit area and is reported in dyne/cm or mN/m.

IFT is an important parameter in chemical, petroleum and petrochemical science and engineering (Aranda-Bravo et al., 2008). It plays an important role in separation processes, multiphase flow, fluid transportation, formation and stability of emulsions and reservoir engineering processes like enhanced oil recovery processes, fluid saturation distribution, fluid contacts and recovery mechanisms (Aranda-Bravo et al., 2008; Bahramian and Danesh, 2004; Danesh, 1998; Jasper and Duncan, 1967; Kahl et al., 2003; Kim and Burgess, 2001).

IFT between pure hydrocarbons and water is very important for liquid-liquid extraction processes and hydrocarbon stream sweetening processes in petroleum and petrochemical industries (Aranda-Bravo et al., 2008; Kahl et al., 2003). The role of IFT has also been acknowledged in understanding hydrocarbon-water emulsion properties and behavior that usually occurs in environment (Demond and Lindner, 1993).

This property can also be implemented in modeling and theoretical works that are done on the hydrocarbon-water interface properties and behavior (Kahl et al., 2003). Therefore accurate quantification and determination of the IFT between pure hydrocarbons and water could be highly desirable.

The most accurate way for determination of interfacial tension between two phases like hydrocarbon and water is to measure it experimentally but it is highly unlikely to measure it under all operating conditions. Besides, experimental measurement of IFT are often time consuming and expensive making it a difficult task when IFT value is required immediately especially in engineering calculations (Demond and Lindner, 1993).

In this connection, theoretical models and empirical correlations have been developed to predict IFT value between pure hydrocarbons and water from known phase parameters. Theoretical models for prediction of the interfacial tension such as those developed by Antonoff (Kim and Burgess, 2001), Donahue and Bartell (1952), Girifalco and Good (1957), Fowkes (1963), Pliskin and Treybal (1966), Paul and Chazal (1969), Fu et al. (1986), Boudh-Hir and Mansoori (1991), Zuo and Stenby (1998), Bahramian and Danesh (2004), Wang and Anderko (2013) are based on theory which in some cases provide only a rough estimate and thus are accompanied by some inaccuracies.

Some of these models may even require some advanced phase properties in their calculations like: partial molar surface area (Bahramian and Danesh, 2004), van der Waals surface area (Fu et al., 1986) and adsorption equilibrium constants (Wang and Anderko, 2013) which in turn introduce more complexity and makes them less popular in engineering calculations.

Some empirical correlations have also been developed for prediction of interfacial tension between pure hydrocarbons and water. They appear to be much simpler than most of the aforementioned theoretical models and mostly require some