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Review article

Viscosity models for pure hydrocarbons at extreme conditions: A review and comparative study

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ABSTRACT

Viscosity is a critical fundamental property required in many applications in the chemical and oil industries. In this review the performance of seven select viscosity models, representative of various predictive and correlative approaches, is discussed and evaluated by comparison to experimental data of 52 pure hydrocarbons including straight-chain alkanes, branched alkanes, cycloalkanes, and aromatics. This analysis considers viscosity data to extremely high-temperature, high-pressure conditions up to 573 K and 300 MPa. Unsatisfactory results are found, particularly at high pressures, with the Chung-Ajlan-Lee-Starling, Pedersen-Fredenslund, and Lohrenz-Bray-Clark models commonly used for oil reservoir simulation. If sufficient experimental viscosity data are readily available to determine model-specific parameters, the free volume theory and the expanded fluid theory models provide generally comparable results that are superior to those obtained with the friction theory, particularly at pressures higher than 100 MPa. Otherwise, the entropy scaling method by Lötgering-Lin and Gross is recommended as the best predictive model.

1. Introduction

The knowledge of the viscosity over wide ranges of temperature, pressure, and composition is required in many petroleum and chemical engineering disciplines, including the estimation of recoverable petroleum within a reservoir, the calculation of flow rates in porous media or wellbores, the forecast of production profiles of petroleum reservoirs, and the design of transport equipment and pipelines. One way to obtain this important property is through experimental measurements. However, direct viscosity measurements for every encountered fluid at all conditions of interest are not only expensive and time-consuming but also extremely difficult and sometimes impossible to obtain especially at high-temperature, high-pressure (HTHP) conditions. Molecular dynamics simulations [1] offer an alternative approach to generating pseudo-experimental viscosity data to supplement real experimental data where experiments are difficult. In general, when performing molecular dynamic simulations, the molecular description is simplified to reduce the computational time, and hence the predicted viscosities are typically only within an order-of-magnitude of experimental values. This approach is currently not commonly accepted by industry [2,3]. Nevertheless, the molecular dynamic simulations can provide valuable insight into the viscosity behavior. Furthermore, with the rapid advances in computing technology, the use of molecular dynamics simulations for engineering purposes is expected to gain more acceptance in the industry.

Reliable viscosity models provide a means for the prediction and correlation of viscosity. The theory of gas viscosity at low pressures is well established with the kinetic theory of the gases, and hence, there are some accurate theoretical models and correlations for the estimation of viscosity of gases. On the other hand, the viscosity theory of liquids is still in need of further development due to complications caused by the intermolecular forces between the molecules [4]. Thus, there is no consensus concerning the mechanism of momentum transfer in liquids and there is no widely accepted simple theoretical method for predicting liquid viscosities. In fact, most viscosity estimation techniques used with liquids are empirical or semi-empirical. Hence, there are many models and correlations in the literature for the estimation of gas and liquid viscosities. Several review articles and books are available on the viscosity of gases and dense fluids including those of Poling et al. [4], Monnery et al. [2], Mehrotra et al. [5], Millat et al. [6], Viswanath et al. [7], and Assael [8].

Various classifications of viscosity models have been proposed, such as the categorization into theoretical, semi-theoretical, and empirical methods. Theoretical models are purely predictive in form, whereas

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Nomenclature

Abbreviations

AAD%	Average absolute Deviation, %
API	American Petroleum Institute
APR	Advanced Peng-Robinson
ASTM	American Society for Testing and Materials
BWR	Benedict-Webb-Rubin
MBWR	Modified Benedict-Webb-Rubin
CALS	Chung-Ajlan-Lee-Starling
CS	Corresponding States
CS-PR	Corresponding States-Pedersen and Fredenslund
ECLIPSE	Exploration Consultants Limited Implicit Program for Simulation Engineering
ECN	Effective Carbon Number
EFT	Expanded Fluid Theory
EFT-YS	Expanded Fluid Theory-Yarranton and Satyro
EoS	Equation of State
ES-LG	Entropy Scaling-Lötgering-Lin and Gross
FT	Friction Theory
FVT	Free-Volume Theory
G-C	Group-Contribution
HTHP	High-Temperature, High-Pressure
JST	Jossi-Stiel-Thodos model
LBC	Lohrenz-Bray-Clarke model
MD	Maximum Deviation
PC-SAFT	Perturbed-Chain Statistical Associating Fluid Theory
PCP-SAFT	Perturbed-Chain Polar Statistical Associating Fluid Theory
PR	Peng-Robinson
PRSV	Peng-Robinson- Stryjek-Vera
PT	Patel-Teja
PVT	Pressure-Volume-Temperature
RHS	Rough Hard Sphere
SBWR	Soave-Benedict-Webb-Rubin
SAFT	Statistical Associating Fluid Theory
SHS	Smooth Hard Sphere
SRK	Soave-Redlich-Kwong
TRAPP	TRAnsport Properties Prediction
UNIQUAC	UNIversal QUAsi-Chemical
VTF	Vogel-Tammann-Fulcher
VW	Vesovic-Wakeham model

Subscripts/superscripts

c	critical
cal	calculated
CE	Chapman-Enskog
exp	experimental
gc	group-contribution
i	component "*i*"
id	ideal
j	component "*j*"
mix	mixture
mol	molar
molec	molecular
n	normal
R	reference
r	reduced
res	residual

Latin letters

A	molar Helmholtz free energy, J·mol^{-1}
B	unitless parameter characteristic of the free-volume overlap, –
B_F	material-specific parameter, –
c_2	fitting parameter in EFT model, –
c_3	pressure dependency parameter in EFT model, kPa^{-1}
c_4	pressure dependency parameter in EFT model, –
E	molar energy, J·mol^{-1}
E_0	barrier energy, J·mol^{-1}
F_c	correction factor of dilute gas viscosity, –
f_v	free-volume fraction, –
g^E	molar excess Gibbs free energy, J·mol^{-1}
H	molar enthalpy, J·mol^{-1}
$\hbar$	Planck's constant, $6.626070040 \times 10^{-34}$ J·s
k_B	Boltzmann's constant, $1.38064852 \times 10^{-23}$ J·K^{-1}
l	characteristic molecular length, Å
L	average characteristic molecular, Å
M	molecular mass, g·mol^{-1}
m	mass, g
m	segment number, –
N	number of data points, –
N_A	Avogadro's number, $6.022140857 \times 10^{23}$ mol^{-1}
P	pressure, Pa
P_a	van der Waals attractive pressure term, Pa
P_{disp}	dispersive pressure, Pa
P_{hc}	hard-chain pressure, Pa
P_r	van der Waals repulsive pressure term, Pa
R	universal gas constant, 8.3144598 J·mol^{-1}·K^{-1}
s	molar entropy, J·mol^{-1}·K^{-1}
T	temperature, K
V	molar volume, cm^{3}·mol^{-1}
V_0	molar close-packed volume, cm^{3}·mol^{-1}
v_f	volume of free-space, cm^{3}·mol^{-1}
v_0	hard-core volume, cm^{3}·mol^{-1}
X	mole fraction, –
Z	compressibility factor, –

Greek letters

α	corresponding states rotational coupling coefficient, –
α	energy parameter, J·mol^{-1}·m^{3}·kg^{-1}
α	viscosibility, Pa^{-1}
β	correlating parameter between viscosity and fluid expansion, –
γ	thermodynamic scaling parameter, –
$\Delta\eta$	residual viscosity, mPa·s
ε	intermolecular potential attractive energy well depth, J
ε	segment energy parameter, J
ζ	free-volume friction coefficient, kg·s^{-1}
η	dynamic viscosity, mPa·s
η_0	dilute gas viscosity, mPa·s
θ	energy shape factor, –
κ_a	linear attractive viscous friction coefficient, –
κ_{aa}	quadratic attractive viscous friction coefficient, –
κ_r	linear repulsive viscous friction coefficient, –
κ_{rr}	quadratic repulsive viscous friction coefficient, –
κ_{rrr}	third-order repulsive friction coefficient, –
κ	association parameter, –
μ	dipole moment, debye
μ_r	reduced dipole moment, –
ν	kinematic viscosity, mm^{2}·s^{-1}
φ	dimensionless scaling parameter, –
ξ	viscosity reducing parameter
ρ	density, kg·m^{-3}
ρ_s^*	compressed state density, kg·m^{-3}
ρ_s^0	compressed state density in vacuum, kg·m^{-3}
σ	collision or hard-sphere diameter, Å