Characterization Scheme for Property Prediction of Fluid Fractions Originating from Biomass - DTU Orbit (08/11/2017)

Characterization Scheme for Property Prediction of Fluid Fractions Originating from Biomass

The composition of industrial fluids is often very difficult to identify from the molecular point of view. In the petroleum industry, the use of the so-called “pseudo-components” is commonly accepted in process modeling, and various approaches exist to determine and/or construct them. We have identified and summarized four such approaches, generally based on experimental information such as boiling temperature and density. Fluids that originate from biomass, however, cannot be treated using only volatility, because of the highly polar character and the high molecular weight of its components, resulting in highly nonideal phase equilibrium behavior. In this work, it is proposed to use a more complete set of experimental descriptors in order to determine the chemical structure of an unknown fluid cut. The definition of such a representative molecule (surrogate) makes it possible to use group contribution or other predictive tools for property calculations or characteristic parameters of an equation of state. In order to achieve this goal, a large database of monofunctional molecules (including alcohols, n-aliphatic acids, aldehydes, ketones, aliphatic ethers, esters, n-alkylbenzenes, and alkanes) has been constructed, which contains a number of descriptors originating from analytical measurements. Using physical insight on the molecular interactions, an algorithm is proposed that uses five descriptors (molecular weight, liquid molar volume, viscosity, refractive index, and dielectric constant) in order to reconstruct a representative molecule.

General information

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, IFP Energies nouvelles
Authors: Nguyen, T. (Ekstern), de Hemptinne, J. (Ekstern), Creton, B. (Ekstern), Kontogeorgis, G. M. (Intern)
Pages: 7230−7241
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Energy and Fuels
Volume: 29
Issue number: 11
ISSN (Print): 0887-0624
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.05
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2

Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes
Web of Science (2000): Indexed yes
Original language: English
DOIs:
10.1021/acs.energyfuels.5b00782
Source: FindIt
Source-ID: 2281549673
Publication: Research - peer-review › Journal article – Annual report year: 2015