

## Accepted Manuscript

A review of molecular simulation applied in vapor-liquid equilibria (VLE) estimation of thermodynamic cycles

Xianhua Nie, Li Zhao, Shuai Deng, Wen Su, Yue Zhang



PII: S0167-7322(18)32186-X  
DOI: doi:[10.1016/j.molliq.2018.05.101](https://doi.org/10.1016/j.molliq.2018.05.101)  
Reference: MOLLIQ 9156  
To appear in: *Journal of Molecular Liquids*  
Received date: 26 April 2018  
Revised date: 20 May 2018  
Accepted date: 22 May 2018

Please cite this article as: Xianhua Nie, Li Zhao, Shuai Deng, Wen Su, Yue Zhang , A review of molecular simulation applied in vapor-liquid equilibria (VLE) estimation of thermodynamic cycles. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:[10.1016/j.molliq.2018.05.101](https://doi.org/10.1016/j.molliq.2018.05.101)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# **A review of molecular simulation applied in vapor-liquid equilibria (VLE) estimation of thermodynamic cycles**

Xianhua Nie, Li Zhao \*, Shuai Deng, Wen Su, Yue Zhang

Key Laboratory of Efficient Utilization of Low and Medium Grade Energy (Tianjin University), MOE, Tianjin University, Tianjin 300072, China

\* Corresponding author. Tel: 86-22-27890051; Fax: 86-22-27404188.

E-mail: jons@tju.edu.cn (L. Zhao).

## **Abstract**

Thermodynamic cycles such as the organic Rankine cycle (ORC), heat pump cycles and refrigeration cycles are flourishing in both industrial and domestic fields. As a carrier of energy conversion among these cycles, working fluids are considered to be a critical factor affecting the thermal performance. Therefore, studies on their thermophysical properties, particularly VLE, attract increasingly attentions of researchers. However, in terms of researches on some mixed working fluids and new working fluids, some conventional methods are limited because of the lack of experimental data. To solve the dilemma, the molecular simulation (MS) was developed and gradually became an efficient and powerful tool for thermodynamic cycles' analyses. In the present work, a comprehensive review on applications of MS for thermodynamic cycles is presented, and analyses focus on VLE of working fluids. The review first covers the state of the art of MS, including a brief introduction of theoretical

Download English Version:

<https://daneshyari.com/en/article/7841995>

Download Persian Version:

<https://daneshyari.com/article/7841995>

[Daneshyari.com](https://daneshyari.com)