Fluid Phase Equilibria 475 (2018) 64–76

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.elsevier.com/locate/fluid

Application of the unscented transform in the uncertainty propagation of thermodynamic model parameters

Hesam Ahmadian Behrooz*, Mohammad Hoseini

Chemical Engineering Faculty, Sahand University of Technology, Tabriz, Iran

ARTICLE INFO

Article history:
Received 21 March 2018
Received in revised form
25 July 2018
Accepted 25 July 2018
Available online 27 July 2018

Keywords:
Uncertainty analysis
Unscented transform
Monte-Carlo
Binary interaction parameter
Cubic equations of state

ABSTRACT

The choice of an appropriate thermodynamic model is one of the critical concerns in the chemical process simulation problems. After the selection of the most appropriate thermodynamic model, the uncertainties associated with the parameters of the model should be taken into account and the effects of such uncertainties should be addressed in the chemical plant design.

In this work, the assumption of normal probability distributions for thermodynamic model parameters is coupled with unscented transform for efficient uncertainty propagation and obtaining probabilistic characteristics of output variables of the simulation model. The proposed methodology can be used easily when the input-output representation of the system such as process simulators are used as the modeling tool of the chemical processes. The law sampling points required in the unscented transform formulation can considerably reduce the computational burden while an acceptable accuracy compared to Monte Carlo techniques can be obtained. The methodology is illustrated by two case studies.

1. Introduction

Process simulators provide a powerful tool for chemical engineers in the steady state design, dynamic simulation and control system design of the chemical processes. Selection of an appropriate thermodynamic model is one of the critical issues that should be addressed carefully in order to obtain acceptable simulation results. Commercial process simulators such as Aspen Plus or Aspen Hysys contain a wide range of built-in thermodynamic models and the user should have an adequate understanding of the thermodynamics and thermodynamic models to make the right choice. Selection of the thermodynamic models for an adequate process simulation is affected by numerous factors, such as temperature, pressure and polarity of the components while various types of equations of state are introduced for electrolyte systems [1]. Despite the fact that some guidelines and heuristics are available to help the user in dealing with the problem, however, comparison of the simulation results with experimental data can only validate the model. In some cases, specific models are also available for special processes such as gas sweetening processes.

It is stated that thermodynamics and process simulation are inseparable components of a successful simulation [2]. Even after the selection of a proper thermodynamic model, the uncertainty of the parameters that appear in the model can influence the quality of the results and predictions. For example, the binary interaction parameters (BIPs) along with the pure component constants such as acentric factors (ω) and critical temperatures (T_c), pressures (P_c) and volumes (V_c) are required when the Peng–Robinson [3] (PR) equation of state (EOS) is chosen for vapor-liquid equilibrium (VLE) calculations of a hydrocarbon mixture.

Pure component constants are either obtained experimentally or estimated using many methods proposed in the literature such as group contribution methods in cases where such experimental data are not at hand or experimental determination of their values can be challenging [4]. These estimation methods are on the basis of the chemical structure of the molecules [5,6]. BIPs are calculated from experimental data or estimated using binary interaction predictive models [7,8] as well.

Pure component constants or mixture properties that appear in the thermodynamic model will introduce some levels of uncertainty in the simulation results if they are provided on the basis of experimental data or an estimation method. The issue can be more challenging in the cases where multiple data are reported for a single parameter. For example, various values are reported for the limiting activity coefficient of a specific solute in a solvent obtained using different experimental methods [9,10].

* Corresponding author.
E-mail address: ahmadian@sut.ac.ir (H. Ahmadian Behrooz).

https://doi.org/10.1016/j.fluid.2018.07.025
0378-3812/

The sensitivity of a property of interest to the parameters of the thermodynamic model can be substantial or negligible depending on the type of components that are present in the system. Even for the latter case, considering the fact that VLE calculations are repeated many times and the uncertainties are propagated through the system in the simulation of a large scale process, the final results might suffer from notable lack of precision. For example, in the simulation of a multicomponent distillation column, VLE flash calculation are carried out sequentially tray-to-tray and the purity of the top and bottom products might be estimated with a notable uncertainty.

The input parameters of an EOS like critical temperatures, critical pressures, acentric factors or BIPs are provided in the process simulators without the corresponding uncertainty data. Accordingly, the uncertainty of the parameters of the thermodynamic model originating either from the experimental error or the error in the results of the estimation techniques may lead to large uncertainties in the simulation results. Therefore, for determining a safety margin in regard to the uncertainty of the thermodynamic model parameters, it is necessary to consider an overdesign factor [11]. However, other systematic methods of uncertainty propagation can help the designer in the analysis of the effects of the uncertain input parameters on the calculated parameters. For example, the model parameters whose uncertainty strongly influences the results of the simulation can be identified.

Uncertainty analysis is required in many fields of engineering like chemical engineering for experimental data analysis and simulation studies [12]. Many studies have been performed in the field of uncertainty analysis and have explored the effects of the uncertainties of the thermodynamic models on the accuracy of the process design.

In the work by Vasquez and Whiting [13], the binary parameters of the NRTL activity coefficient model were estimated using different experimental data. The results of the uncertainty analysis using random Monte Carlo simulation (MCS) [14] coupled with the Latin Hypercube Sampling (LHS) technique reveals that the effects of the uncertainty of the estimated binary parameters originating from various experimental data sets can be notable on the simulation results of a liquid-liquid extractor. Effect of the uncertainties in the estimated physical properties of hot-gas mixtures at high temperatures on heat exchanger design was studied by Clarke et al. [15] using MCS analysis with LHS. A Linear and a non-linear technique for sensitivity analysis were used in the uncertainty analysis of a multi-tubular fixed-bed catalytic reactor design and operability [16]. In the work by Cadoret et al. [17], different approaches such as data regression, UNIFAC and COSMO-SAC predictive models were applied to estimate the parameters of the NRTL model. The effects of the resulting uncertainty in the thermodynamic model on the process design were also studied in a distillation separation process for a four component mixture using Aspen Plus simulator. Sin et al. [18] performed the uncertainty analysis for an antibiotic production plant where the MCS procedure was used to build the output distribution. The analysis showed that the output uncertainty level in the predicted antibiotic and off-gas CO2 was more notable compared to biomass, glucose, ammonium and base-consumption.

Hajipour and Satyro [11] used NIST's Thermo Data Engine (TDE) [19] to develop a database of critical constants, acentric factors, interaction parameters along with their uncertainties for hydrocarbons commonly encountered in natural gas processing industry [20]. A Monte Carlo procedure was adopted by Frutiger et al. [21] to propagate the parameter uncertainties of the Soave–Redlich–Kwong [22] (SRK) and PC-SAFT EOS from measured data to obtain their effects on the uncertainty of cycle power production in an organic Rankine cycle. The methodology has been also used for working fluid selection for organic Rankine cycles [23]. Burger et al. [24] proposed a perturbation approach for the liquid phase fugacity coefficients. Mathias [25] has proposed an activity-coefficient perturbation scheme and the idea was elaborated for VLE [25] and liquid-liquid equilibrium [26] analysis. The reliability aspects associated with a proton exchange membrane fuel cell stack was studied by Noguer et al. [27] using MCS method.

Our study focuses on the efficient propagation of the thermodynamic model parameter uncertainties using unscented transform (UT). Formulation with a low number of sampling points and ease of implementation when process simulators are used as the modeling tool of chemical processes are the advantages of the proposed method.

In this paper, the unscented transform is first introduced as an efficient uncertainty propagation tool for thermodynamic applications in Section 2 and the procedure is discussed in detail. In Section 3, the methodology is applied to two case studies to elaborate the proposed method. The effects of the uncertainties of the thermodynamic models are discussed where the results are compared with MCS method and the possibility of increasing the robustness of the process under the thermodynamic model parameters uncertainty is also shown. Finally, in Section 4 the conclusions are drawn.

2. Uncertainty propagation

The uncertainty associated with process simulation can originate from different sources including: 1) modeling uncertainties where a simplified mathematical model is derived for the real system, 2) stochastic uncertainties originating from various noise sources imposed on the system and 3) input uncertainties due to lack of knowledge about the fixed parameters of the model [23,28].

All experimental data have some level of experimental uncertainty and appropriate methodology to deal with the experimental uncertainty of the thermodynamic model parameters in process simulation and design must be adopted. First, the uncertainty levels corresponding to each parameter should be quantified. The appearance of thermodynamic model parameters in the simulation model of the plant will be reflected in the output parameters as well and an efficient uncertainty analysis tool is required to estimate the uncertainty level of the system desired output variables.

A schematic representation of the model we are dealing with is shown in Fig. 1 where x is defined as the stochastic input parameters vector, r as the deterministic input parameters vector, y as the output parameters vector and g as the function that relates the input vector to the output vector. The system can be also represented by Eq. (1) where g is the computer simulation model of the system.

$$y = g(x, r) \tag{1}$$

Despite the fact that analytical tools can be used for obtaining the probabilistic characteristics of the output random variables for known probabilistic characteristics of input random variables, however, analytical complexity motivates approximate methods [29]. For example, probability density function (PDF) of the dependent variables can be obtained on the basis of the PDF corresponding to the uncertain input parameters using numerical methods such as orthogonal collocation method for the multidimensional probability integral calculations [30]. However, the curse of the dimensionality makes these methods less efficient in the cases with many uncertain parameters.

There are several methods available for propagating uncertainty of the stochastic input vector x which corresponds to thermodynamic model parameters subject to uncertainty when a computer simulation model of the system is developed. These characterization