

Accepted Manuscript

Parameter Estimation for Cubic Equations of State Models Subject to Sufficient Criteria for Thermodynamic Stability

Moll Glass, Hatim Djelassi, Alexander Mitsos

PII: S0009-2509(18)30604-3
DOI: <https://doi.org/10.1016/j.ces.2018.08.033>
Reference: CES 14448

To appear in: *Chemical Engineering Science*

Received Date: 3 March 2018
Revised Date: 22 July 2018
Accepted Date: 14 August 2018

Please cite this article as: M. Glass, H. Djelassi, A. Mitsos, Parameter Estimation for Cubic Equations of State Models Subject to Sufficient Criteria for Thermodynamic Stability, *Chemical Engineering Science* (2018), doi: <https://doi.org/10.1016/j.ces.2018.08.033>

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.



1 **Parameter Estimation for Cubic Equations of State**
2 **Models Subject to Sufficient Criteria for Thermodynamic**
3 **Stability**

4 Moll Glass^a, Hatim Djelassi^b, and Alexander Mitsos^c

5 ^{a,b,c} RWTH Aachen University

6 AVT - Aachener Verfahrenstechnik

7 Process Systems Engineering

8 Forckenbeckstraße 51

9 D - 52074 Aachen, Germany

10 ^a moll.glass@avt.rwth-aachen.de, ^b hatim.djelassi@avt.rwth-aachen.de,

11 ^c corresponding author: amitsos@alum.mit.edu, fax +49 (0) 241 80 - 92326, phone

12 +49 (0) 241 80 - 94704.

13 **Abstract:** A formulation for parameter estimation in cubic equations of state
14 (CEOS) models for phase equilibrium thermodynamics is proposed. This formu-
15 lation *guarantees* for the regressed parameters that the predicted mole fractions
16 correspond to stable equilibria, when standard methods fail and demonstrably
17 entail erroneous process simulation results. The present formulation overcomes
18 these deficiencies, which is predicated on a bilevel structure extending Mitsos
19 et al. (*Chem. Eng. Sci.*, 64:548-559, 2009). That is, an upper-level (parameter
20 fitting) problem is minimized, subject to multiple lower-level problems, which
21 encode thermodynamic stability. The CEOS constitutes an equality constraint
22 on the lower level, which adds to the difficulty of the bilevel program. For the
23 VLE of C₅H₁₂/H₂S, it is demonstrated that the method permits an acceptable
24 fit with physically sensible CEOS root values. Thus, the regressed parameter
25 values may be applied to, e.g., process simulation.

26 **Keywords:** cubic equation of state, data regression, bilevel program, tangent
27 criterion, false liquid-liquid split

Abbreviations: bilevel program (BLP), cubic equation of state (CEOS), equality constraint (EC), inequality constraint (IC), Karush-Kuhn-Tucker (KKT), lower bound (LBD), lower-bounding problem (LBP), left-hand side (LHS), Linear Independence Constraint Qualification (LICQ), liquid-liquid equilibrium (LLE), lower-level problem (LLP), mixed-integer nonlinear program (MINLP), nonlinear program (NLP), Non-Random Two Liquid (NRTL), Perturbed Chain - Statistical Associated Fluid Theory (PC-SAFT), Peng-Robinson CEOS (PR), right-hand side (RHS), Redlich-Kwong CEOS (RK), semi-infinite program (SIP), Soave-Redlich-Kwong CEOS (SRK), tangent plane distance function (TPD), Trebble-Bishnoi CEOS (TB), upper bound (UBD), Universal Quasichemical Functional Group Activity Coefficients (UNIFAC), vapor-liquid(-liquid) equilibrium (VL(L)E), upper critical solution temperature (UCST)

Download English Version:

<https://daneshyari.com/en/article/11000256>

Download Persian Version:

<https://daneshyari.com/article/11000256>

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