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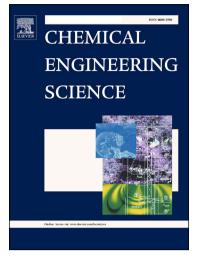
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Parameter Estimation for Cubic Equations of State Models Subject to Sufficient Criteria for Thermodynamic Stability

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- ² Models Subject to Sufficient Criteria for Thermodynamic
- ³ Stability
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Abstract: A formulation for parameter estimation in cubic equations of state 13 (CEOS) models for phase equilibrium thermodynamics is proposed. This formu-14 lation guarantees for the regressed parameters that the predicted mole fractions 15 correspond to stable equilibria, when standard methods fail and demonstrably 16 entail erroneous process simulation results. The present formulation overcomes 17 these deficiencies, which is predicated on a bilevel structure extending Mitsos 18 et al. (Chem. Eng. Sci., 64:548-559, 2009). That is, an upper-level (parameter 19 fitting) problem is minimized, subject to multiple lower-level problems, which 20 encode thermodynamic stability. The CEOS constitutes an equality constraint 21 on the lower level, which adds to the difficulty of the bilevel program. For the 22 VLE of C_5H_{12}/H_2S , it is demonstrated that the method permits an acceptable fit with physically sensible CEOS root values. Thus, the regressed parameter 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)

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