Automated calculation of complete Pxy and Txy diagrams for binary systems

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An algorithm for the calculation of global phase equilibrium diagrams has been recently developed [M. Cismondi, M.L. Michelsen, Global phase equilibrium calculations: critical lines, critical end points and liquid-liquid-vapour equilibrium in binary mixtures, J. Supercrit. Fluids 39 (2007) 287-295]. It integrates the calculation of critical lines, liquid-liquid-vapour (LLV) lines and critical end points, and was implemented in the software program GPEC: global phase equilibrium calculations [M. Cismondi, D.N. Nunez, M.S. Zabaloy, E.A. Brignole, M.L. Michelsen, J.M. Mollerup, GPEC: a program for global phase equilibrium calculations in binary systems, in: Proceedings of the CD-ROM EQUIFASE 2006, Morelia, Michoacan, Mexico, October 21-25, 2006; www.gpec.plapiqui.edu.ar]. In this work we present the methods and computational strategy for the automated calculation of complete Pxy and Txy diagrams in binary systems. Being constructed from the points given by the global phase diagram at a specified temperature or pressure, their calculation does not require the implementation of stability analysis. We illustrate the application of the algorithm through a variety of Pxy and Txy diagrams generated using the RK-PR EOS.

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