



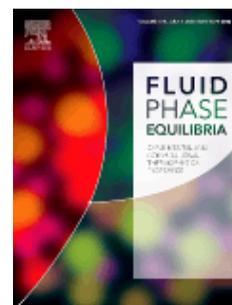
FLUID PHASE EQUILIBRIA

An International Journal

AUTHOR INFORMATION PACK

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DESCRIPTION

Fluid Phase Equilibria publishes high-quality papers dealing with experimental, theoretical, and applied research related to equilibrium and transport properties of fluids, solids, and interfaces. Subjects of interest include physical/phase and chemical equilibria; equilibrium and nonequilibrium thermophysical properties; fundamental thermodynamic relations; and stability. The systems central to the journal include pure substances and mixtures of organic and inorganic materials, including polymers, biochemicals, and surfactants with sufficient characterization of composition and purity for the results to be reproduced. Alloys are of interest only when thermodynamic studies are included, purely material studies will not be considered. In all cases, authors are expected to provide physical or chemical interpretations of the results.

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Editorial and Introduction

Editorial

New procedures for articles reporting thermophysical properties

Fluid Phase Equilibria, along with other journals in the field, established collaboration with the Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST) in 2009 for the purpose of ensuring the quality of published experimental data. In a joint statement [1], the editors of the five journals involved set out the rationale for the cooperation in terms of helping to ensure that authors and reviewers were made aware of any previously-published literature values for the properties and systems in question. The process involved NIST 'capturing' the new experimental data, comparing it against existing values in the NIST data archive and providing a report that: (a) listed relevant literature sources; and (b) highlighted any obvious discrepancies in the new data.

In order to streamline the process and to further enhance the quality of published articles, we are now introducing one change to the way in which the NIST cooperation is implemented. Effective in February 2013, responsibility for preparing a *Literature Report* will shift from NIST to the submitting authors. Submitting authors will be able to prepare their own *Literature Report* by using *ThermoLit*, a publicly available (<http://trc.nist.gov/thermolit/>) program. This will eliminate NIST's role in providing this report, and thus speed the review process and provide added benefit to authors who will have literature citation results on hand at a stage when they can do the most good. Please, note that use of *ThermoLit* is designed as an aid to the traditional required literature review and must not be used as a substitute.

NIST will continue to provide a data evaluation at the end of the review process, immediately prior to final acceptance of the article. This data evaluation will compare the reported experimental data with that existing in the NIST Data Archive and highlight any unexpectedly large discrepancies, such as those arising from typographical errors. Though the data evaluation step has not changed, we will use this opportunity for a reminder that experimental results and their uncertainties must be tabulated in the way described in the Guide for Authors. A key feature is that tables be self-contained and include the uncertainties of all reported quantities (variables, constraints, and properties). In addition, we have incorporated new standards relating to the description of chemical samples and we encourage authors to present details of their samples in an easily-readable tabular form. To assist authors, a large number of example tables have been prepared by NIST and are available (<http://trc.nist.gov/FPE-Support.html>).

The new procedures will provide literature citations to authors before submission of their manuscript and speed the review process. Indeed, authors are encouraged to use *ThermoLit* in advance of experiments to help minimize duplication of effort. In 2012, new IUPAC guidelines for the reporting of phase equilibrium measurements were published (Pure Appl. Chem. 2012, 84(8), 1785-1813), and the requirements of this journal are consistent with these recommendations. Prior to submission, authors are strongly encouraged to review a checklist based on these recommendations, which is available (<http://trc.nist.gov/FPE-Support.html>). We are certain that the new Literature Report tool and the procedures described here will further enhance the already high quality of articles published in *Fluid Phase Equilibria*.

References

1. P.T. Cummings, Th.W. de Loos, J.P. O'Connell, *Fluid Phase Equilibria* 276 (2009) 1165-1166.

Aims and Scope

Fluid Phase Equilibria publishes high-quality papers dealing with experimental, theoretical, and applied research related to equilibrium and transport properties of fluids, solids, and interfaces. Subjects of interest include physical/phase and chemical equilibria; equilibrium and nonequilibrium thermophysical properties; fundamental thermodynamic relations; and stability. The systems central to the journal include pure substances and mixtures of organic and inorganic materials, including polymers, biochemicals, and surfactants with sufficient characterization of composition and purity for the results to be reproduced. In all cases, enough detail must be given to permit independent verification, and authors are also expected to provide physical or chemical interpretations of the results.

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Theoretical studies can include equations of state; correlations or predictive models; molecular dynamics and Monte Carlo simulations; statistical thermodynamics; quantum chemistry; and applied mathematical and computational approaches. Research reporting new theories and models is expected to show adequate comparisons of predictive ability and accuracy with both applicable data and contemporary existing models. Contributions on artificial neural networks and similar approaches will only be considered when full details of the methodology are provided and comparisons of accuracy are made with existing physically-based models, or if no thermodynamic models are available.

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[3] W. Strunk Jr., E.B. White, *The Elements of Style*, fourth ed., Longman, New York, 2000.

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[4] G.R. Mettam, L.B. Adams, How to prepare an electronic version of your article, in: B.S. Jones, R.Z. Smith (Eds.), *Introduction to the Electronic Age*, E-Publishing Inc., New York, 2009, pp. 281–304.

Reference to a website:

[5] Cancer Research UK, Cancer statistics reports for the UK. <http://www.cancerresearchuk.org/aboutcancer/statistics/cancerstatsreport/>, 2003 (accessed 13 March 2003).

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