A New Group Contribution Method For The Estimation Of

Process Systems Engineering brings together the international community of researchers and engineers interested in computing-based methods in process engineering. This conference highlights the contributions of the PSE community towards the sustainability of modern society and is based on the 13th International Symposium on Process Systems Engineering PSE 2018 event held San Diego, CA, July 1-5 2018. The book contains contributions from academia and industry, establishing the core products of PSE, defining the new and changing scope of our results, and future challenges. Plenary and keynote lectures discuss real-world challenges (globalization, energy, environment and health) and contribute to discussions on the widening scope of PSE versus the consolidation of the core topics of PSE. Highlights how the Process Systems Engineering community contributes to the sustainability of modern society Establishes the core products of Process Systems Engineering Defines the future challenges of Process Systems Engineering

*Properties of chemical compounds and their mixtures are needed in almost every aspect of process and product design. When the use of experimental data is not possible, one of the most widely used options in the use of property estimation models. Computer Aided Property Estimation for Process and Product Design provides a presentation of the most suitable property estimation models available today as well as guidelines on how to select an appropriate model. Problems that users are faced with, such as: which models to use and what their accuracy is, are addressed using a systematical approach to property estimation. The volume includes contributions from leading experts from academia and industry. A wide spectrum of properties and phase equilibria types is covered, making it indispensable for research, development and educational purposes. * This book presents the latest developments in computational modelling for thermodynamic property estimation. * It combines theory with practice and includes illustrative examples of software applications. * The questions users of property models are faced with are addressed comprehensively.*

In conjunction with top survey researchers around the world and with Nielsen Media Research serving as the corporate sponsor, the Encyclopedia of Survey Research Methods presents state-of-the-art information and methodological examples from the field of survey research. Although there are other "how-to" guides and references texts on survey research, none is as comprehensive as this Encyclopedia, and none presents the material in such a focused and approachable manner. With more than 600 entries, this resource uses a Total Survey Error perspective that considers all aspects of possible survey error from a cost-benefit standpoint.

Prediction of Thermodynamic Properties by Structure-based Group Contribution Approaches

Documentation of the Basis for Selection of Prediction Methods for Organometallic Compounds in Manual for Predicting Chemical Process Design Data

White Fragility

Chemical Structure Generation from the Properties of Pure Organic Compounds

Prediction of Viscosity of Organic Liquid Mixtures by a Group Contribution Method

From Classical and Advanced Mixing Rules to Association Theories

For more than 100 years the Beilstein Handbook has been publishing checked and evaluated data on organic compounds. It has become the major reference book for the chemical and physical properties of organic com pounds. The prediction of these physical properties was the subject of the Beilstein workshop. The ability to predict physical properties is for several reasons of great interest to the Beilstein Institute. It is of primary importance to be able

to check the abstracted data for accuracy and to eliminate simple mistakes like typing errors. Presently all the work whether manuscript writing or evaluation of data is carried out manually. This is very time consuming, with the entry of Beilstein into electronic data gathering and publication, the opportunity for computerized consistency checking has become available. Contrary to belief, when one examines the Beilstein Handbook or Chemical Abstracts there is a dearth of chemical information. There are a great many compounds but few are well defined resulting in large gaps in the information available to the chemist. These information gaps could be filled by using algorithmic methods to estimate the properties of interest. An important question to answer is "What is the chemist's reaction to estimated data?" Will he accept it for use, within limits defined by the method, or will it be unacceptable and therefore detrimental for the data base. However if one could partly fill gaps in the data base the increase in the power of the search techniques would be marked.

Using an applications perspective Thermodynamic Models for Industrial Applications provides a unified framework for the development of various thermodynamic models, ranging from the classical models to some of the most advanced ones. Among these are the Cubic Plus Association Equation of State (CPA EoS) and the Perturbed Chain Statistical Association Fluid Theory (PC-SAFT). These two advanced models are already in widespread use in industry and academia, especially within the oil and gas, chemical and polymer industries. Presenting both classical models such as the Cubic Equations of State and more advanced models such as the CPA, this book provides the critical starting point for choosing the most appropriate calculation method for accurate process simulations. Written by two of the developers of these models, Thermodynamic Models for Industrial Applications emphasizes model selection and model development and includes a useful “which model for which application” guide. It also covers industrial requirements as well as discusses the challenges of thermodynamics in the 21st Century.

Tools for Chemical Product Design: From Consumer Products to Biomedicine describes the challenges involved in systematic product design across a variety of industries

and provides a comprehensive overview of mathematical tools aimed at the design of chemical products, from molecular design to customer products. Chemical product design has become increasingly important over the past decade and includes a wide range of sectors including gasoline additives and blends in the petroleum industry, active ingredients and excipients in the pharmaceutical industry, and a variety of consumer products and specialty chemicals. Traditionally, such products have been designed through trial and error methods, which not only are time-consuming, but more importantly only provide limited knowledge that can be translated into next generation products. Features an impressive collection of contributions from leading researchers in the field Presents the latest tools available across a variety of industries Describes the challenges involved in systematic product design as well as the latest methods for solving such problems Covers a wide range of sectors including gasoline additives and blends in the petroleum industry, active ingredients and excipients in the pharmaceutical industry, and a variety of consumer products and specialty chemicals

Qh-wln New Coding and Decoding Method for Structure of Chemical Compounds

Gas Solubilities by Means of a Group Contribution Method. A Progress Report

From Consumer Products to Biomedicine

The Discipline of Teams

The Properties of Gases and Liquids

Thermodynamic Models for Industrial Applications

According to certain rules the decoding software devoloped in this paper can take chemical substance apart into some function groups automatically. With group contribution method, it is possoble to estimate the physical and chemical properties of certain substance which may be not available in the basic physical and chemical properties database. Combined with graph function of computer it would be helpful to the display of molecular structure. Therefore the coding and decoding mehtod will also play a very important role in the study of substance structure and computer aided molecular design. [Authors' abstract].

J.-P. CALISTE, A. TRUYOL AND J. WESTBROOK The Series, "Data and Knowledge in a Changing World", exemplifies CODATA's primary purpose of collecting, from widely different fields, a wealth of information on efficient exploitation of data for progress in science and technology and making that information available to scientists and engineers. A separate and complementary CODATA Reference Series will present Directories of compiled and evaluated data and Glossaries of data-related terms. The present book "Thermodynamic Modeling and Materials Data Engineering" discusses thermodynamic, structural, systemic and heuristic approaches to the modeling of complex materials behavior in condensed phases, both fluids and solids, in order to evaluate their potential applications. Itwas inspired by the Symposium on

"Materials and Structural Properties" held during the 14th International CODATA Conference in Chambery, France. The quality of the contributions to this Symposium motivated us to present" a coherent book of interest to the field. Updated contributions inspired by Symposium discussions and selections from other CODATA workshops concerning material properties data and Computer Aided Design combine to highlight the complexity of material data issues on experimental, theoretical and simulation levels Articles were selected for their pertinence in three areas. Complex data leading to interesting developments and tools such as: • new developments in state equations and their applications, • prediction and validation of physical and energy data by group correlations for pure compounds, • modeling and prediction of mixture properties.

Must-have reference for processes involving liquids, gases, and mixtures Reap the time-saving, mistake-avoiding benefits enjoyed by thousands of chemical and process design engineers, research scientists, and educators. Properties of Gases and Liquids, Fifth Edition, is an all-inclusive, critical survey of the most reliable estimating methods in use today --now completely rewritten and reorganized by Bruce Poling, John Prausnitz, and John O'Connell to reflect every late-breaking development. You get on-the-spot information for estimating both physical and thermodynamic properties in the absence of experimental data with this property data bank of 600+ compound constants. Bridge the gap between theory and practice with this trusted, irreplaceable, and expert-authored expert guide -- the only book that includes a critical analysis of existing methods as well as hands-on practical recommendations. Areas covered include pure component constants; thermodynamic properties of ideal gases, pure components and mixtures; pressure-volume-temperature relationships; vapor pressures and enthalpies of vaporization of pure fluids; fluid phase equilibria in multicomponent systems; viscosity; thermal conductivity; diffusion coefficients; and surface tension.

A PC-SAFT Group Contribution Method for Polymers

A Statistical Mechanical Group Contribution Method for Calculating Thermodynamic Properties of Fluids

A New Class of Group Contribution Based Property Estimation Methods for Process Modelling and Design

Thermophysical Properties of Chemicals and Hydrocarbons

Thermodynamics of Biochemical Reactions

Molecular Design

Vapor-Liquid Equilibria Using UNIFAC: A Group-Contribution Method focuses on the UNIFAC group-contribution method used in predicting quantitative information on the phase equilibria during separation by estimating activity coefficients. Drawing on tested vapor-liquid equilibrium data on which UNIFAC is based, it demonstrates through examples how the method may be used in practical engineering design calculations. Divided into nine chapters, this volume begins with a discussion of vapor and liquid phase nonidealities and how they are calculated in terms of fugacity and activity coefficients, respectively. It then introduces the reader to the UNIFAC method and how it works, the procedure used in establishing the parameters needed for the model, prediction of binary and multicomponent vapor-liquid equilibria for a large number of systems, the potential of UNIFAC for predicting liquid-liquid equilibria, and how UNIFAC can be used to solve practical distillation design problems. This book will benefit process design engineers who want to reliably predict phase equilibria for designing distillation columns and other separation processes.

Comprises 20 contributions which grew from the August 1996 symposium. Representative paper topics include estimating phase- change enthalpies and entropies, electrostatic-covalent model parameters for molecular modeling, complete basis-set thermochemistry and kinetics, modeling free energies of solvation and transfer, use of density functional methods to compute heats of reaction, and a density functional study of periodic trends in bond energies. Together

the contributions describe all the major methods used for estimating or predicting molecular thermochemistry. Appends information on software and databases for thermochemistry, essential statistical thermodynamics, and worked examples. Annotation copyrighted by Book News, Inc., Portland, OR

The second edition of the Impact Evaluation in Practice handbook is a comprehensive and accessible introduction to impact evaluation for policy makers and development practitioners. First published in 2011, it has been used widely across the development and academic communities. The book incorporates real-world examples to present practical guidelines for designing and implementing impact evaluations. Readers will gain an understanding of impact evaluations and the best ways to use them to design evidence-based policies and programs. The updated version covers the newest techniques for evaluating programs and includes state-of-the-art implementation advice, as well as an expanded set of examples and case studies that draw on recent development challenges. It also includes new material on research ethics and partnerships to conduct impact evaluation. The handbook is divided into four sections: Part One discusses what to evaluate and why; Part Two presents the main impact evaluation methods; Part Three addresses how to manage impact evaluations; Part Four reviews impact evaluation sampling and data collection. Case studies illustrate different applications of impact evaluations. The book links to complementary instructional material available online, including an applied case as well as questions and answers. The updated second edition will be a valuable resource for the international development community, universities, and policy makers looking to build better evidence around what works in development.

13th International Symposium on Process SystemsEngineering - PSE 2018, July 1-5 2018

Encyclopedia of Survey Research Methods

Computer Aided Molecular Design

An Extension of the UNIFAC Group Contribution Method to Distinguish Between Aromatic Isomers

A Group Contribution Method for Liquid Viscosity

Combustible Organic Materials

Thermodynamics of Biochemical Reactions emphasizes the fundamental equations of thermodynamics and the application of these equations to systems of biochemical reactions. This emphasis leads to new thermodynamic potentials that provide criteria for spontaneous change and equilibrium under the conditions in a living cell.

CAMD or Computer Aided Molecular Design refers to the design of molecules with desirable properties. That is, through CAMD, one determines molecules that match a specified set of (target) properties. CAMD as a technique has a very large potential as in principle, all kinds of chemical, bio-chemical and material products can be designed through this technique. This book mainly deals with macroscopic properties and therefore does not cover molecular design of large, complex chemicals such as drugs. While books have been written on computer aided molecular design relating to drugs and large complex chemicals, a book on systematic formulation of CAMD problems and solutions, with emphasis on theory and practice, which helps one to learn, understand and apply the technique is currently unavailable. · This title brings together the theoretical aspects related to

Computer Aided Molecular Design, the different techniques that have been developed and the different applications that have been reported. · Contributing authors are among the leading researchers and users of CAMD · First book available giving a systematic formulation of CAMD problems and solutions

Much of the research on advanced biofuels is devoted to the study of novel chemical pathways for converting nonfood biomass into liquid fuels that can be blended with existing transportation fuels. Many compounds under consideration are not found in the existing fuel supplies. Often, the physical properties needed to assess the viability of a potential biofuel are not available. The only reliable information available may be the molecular structure. Group contribution methods for estimating physical properties from molecular structure have been used for more than 60 years. The most common application is estimation of thermodynamic properties. More recently, group contribution methods have been developed for estimating rate dependent properties including cetane and octane numbers. Often, published group contribution methods are limited in terms of types of function groups and range of applicability. In this study, a new, broadly-applicable group contribution method based on an artificial neural network was developed to estimate cetane number research octane number, and motor octane numbers of hydrocarbons and oxygenated hydrocarbons. The new method is more accurate over a greater range molecular weights and structural complexity than existing group contribution methods for estimating cetane and octane numbers.

Computational Thermochemistry

A Group-Contribution Method

Formulation of Gels and Pastes

Determination and Prediction of Combustion Properties

Theory and Practice

Physico-chemical Constants of Pure Organic Compounds

Compiled by an expert in the field, the book provides an engineer with data they can trust. Spanning gases, liquids, and solids, all critical properties (including viscosity, thermal conductivity, and diffusion coefficient) are covered. From C1 to C100 organics and Ac to Zr inorganics, the data in this handbook is a perfect quick reference for field, lab or classroom usage. By collecting a large - but relevant - amount of information in one source, the handbook enables engineers to spend more time developing new designs and processes, and less time collecting vital properties data. This is not a theoretical treatise, but an aid to the practicing engineer in the field, on day-to-day operations and long range projects. Simplifies research and significantly reduces the amount of time spent collecting

properties data Compiled by an expert in the field, the book provides an engineer with data they can trust in design, research, development and manufacturing A single, easy reference for critical temperature dependent properties for a wide range of hydrocarbons, including C1 to ClOO organics and Ac to Zr inorganics

The New York Times best-selling book exploring the counterproductive reactions white people have when their assumptions about race are challenged, and how these reactions maintain racial inequality. In this “vital, necessary, and beautiful book” (Michael Eric Dyson), antiracist educator Robin DiAngelo deftly illuminates the phenomenon of white fragility and “allows us to understand racism as a practice not restricted to ‘bad people’ (Claudia Rankine). Referring to the defensive moves that white people make when challenged racially, white fragility is characterized by emotions such as anger, fear, and guilt, and by behaviors including argumentation and silence. These behaviors, in turn, function to reinstate white racial equilibrium and prevent any meaningful cross-racial dialogue. In this in-depth exploration, DiAngelo examines how white fragility develops, how it protects racial inequality, and what we can do to engage more constructively.

This research suggests two new group contribution methods to facilitate phase behavior calculation when reliable experimental data are lacking. The first method pertains to the implementation of an updated version of the Elliott and Natarajan method to the Statistical Associating Fluid Theory (SAFT) and Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) equations of state. Shape factor parameters have been correlated for 878 compounds including different variety of families and the parameters from Elliott and Natarajan have been updated to improve accuracy for alcohols. Thereafter, thermodynamic properties such as boiling temperatures and vapor pressures have been predicted. We obtain 36%, 65%, and 32% AAD% in pressures for the ESD, SAFT, and PC-SAFT equations of state. Additionally, we have compared our GC-PC-SAFT to the one by Tihic et al., applying their suggested First-Order and Second-Order groups for 650 non-associating compounds. We observed higher accuracy for our method relative to the Tihic et al. The resulting P AAD% were 53% for Tihic FOG and 42% for Tihic SOG. The second method suggests a new group contribution model for Tb at 760mmHg and Tb at 10 mmHg. These correlations recognize a finite limit in boiling temperature as infinite molecular weight is approached. The availability of two vapor pressures enables straightforward application of the Clausius-Clapeyron equation to estimate boiling temperatures at other points. In the

presented approach, there are 3 parameters and 72 functional groups for each temperature which are regressed through a database consisting of 336 hydrocarbons and 642 non-hydrocarbons. The average absolute percent deviations (AAD%) between the correlated and experimental temperatures are calculated in comparison with Joback-Reid and Gani approaches. We obtain 3.5, 4.7, and 4.1 AAD% in temperature for the present work, Joback, and Gani methods, respectively. Additionally, the accuracy of the present work is evaluated by calculating the vapor pressures from the DIPPR correlation at the predicted temperatures of each model. We obtained 33.2, 104.3 and 48.1 AAD% in pressure for the present work, Joback, and Gani methods. Finally, the accuracy of the presented correlations are tested against Asher and Pankow model, UNIFAC-PL°, for 66 volatile compounds in the temperature range of 290-320 K. For the vapor pressure at the 10mmHg boiling temperature, we obtain 36.9 AAD% for the present work and 94.5 AAD% for the Asher method. Overall, these group contribution methods establish a standard for comparison of more fundamental methods like molecular simulations with transferable potentials. Transferable potentials generally provide accuracy of 10-30AAD% in pressure, but have only been developed for relatively small databases over narrow temperature ranges.

Proceedings of the Beilstein Workshop, 16-20th May, 1988, Schloss Korb, Italy

Process Systems Engineering for Biofuels Development

Prediction and Estimation of Molecular Thermodynamics

Physical Property Prediction in Organic Chemistry

Product Design and Engineering

Tools For Chemical Product Design

The 18th European Symposium on Computer Aided Process Engineering contains papers presented at the 18th European Symposium of Computer Aided Process Engineering (ESCAPE 18) held in Lyon, France, from 1-4 June 2008. The ESCAPE series brings the latest innovations and achievements by leading professionals from the industrial and academic communities. The series serves as a forum for engineers, scientists, researchers, managers and students from academia and industry to: - present new computer aided methods, algorithms, techniques related to process and product engineering, - discuss innovative concepts, new challenges, needs and trends in the area of CAPE. This research area bridges fundamental sciences (physics, chemistry, thermodynamics, applied mathematics and computer sciences) with the various aspects of process and product engineering. The special theme for ESCAPE-18 is CAPE for the Users! CAPE systems are to be put in the hands of end users who need

*functionality and assistance beyond the scientific and technological capacities which are at the core of the systems. The four main topics are: - off-line systems for synthesis and design, - on-line systems for control and operation, - computational and numerical solutions strategies, - integrated and multi-scale modelling and simulation, Two general topics address the impact of CAPE tools and methods on Society and Education. * CD-ROM that accompanies the book contains all research papers and contributions * International in scope with guest speeches and keynote talks from leaders in science and industry * Presents papers covering the latest research, key top areas and developments in Computer Aided Process Engineering*

Covering the whole value chain - from product requirements and properties via process technologies and equipment to real-world applications - this reference represents a comprehensive overview of the topic. The editors and majority of the authors are members of the European Federation of Chemical Engineering, with backgrounds from academia as well as industry. Therefore, this multifaceted area is highlighted from different angles: essential physico-chemical background, latest measurement and prediction techniques, and numerous applications from cosmetic up to food industry. Recommended reading for process, pharma and chemical engineers, chemists in industry, and those working in the pharmaceutical, food, cosmetics, dyes and pigments industries.

In The Discipline of Teams, Jon Katzenbach and Douglas Smith explore the often counter-intuitive features that make up high-performing teams—such as selecting team members for skill, not compatibility—and explain how managers can set specific goals to foster team development. The result is improved productivity and teams that can be counted on to deliver more than just the sum of their parts. Since 1922, Harvard Business Review has been a leading source of breakthrough ideas in management practice. The Harvard Business Review Classics series now offers you the opportunity to make these seminal pieces a part of your permanent management library. Each highly readable volume contains a groundbreaking idea that continues to shape best practices and inspire countless managers around the world.

Computer Aided Property Estimation for Process and Product Design

Computers Aided Chemical Engineering

Development of a Second-order Group Contribution Method for the Estimation of Pure Component Vapor Pressure

Vapor-Liquid Equilibria Using Unifac

Development of a Group Contribution Method for the Prediction of Normal Boiling Points of Non-electrolyte Organic Compounds

Why It's So Hard for White People to Talk About Racism

The combustion properties of organic materials are used to assess their safety specifications. This knowledge is necessary to avoid potentially disastrous fires. The experimental determination of the combustion properties of a new organic compound is laborious and sometimes even impossible. This book describes methods for the determination and prediction of the combustion properties of organic compounds, along with some examples and exercises.

A Group Contribution Method for Estimating Cetane and Octane Numbers

This book is a systematic presentation of the methods that have been developed for the interpretation of molecular modeling to the design of new chemicals. The main feature of the compilation is the co-ordination of the various scientific disciplines required for the generation of new compounds. The five chapters deal with such areas as structure and properties of organic compounds, relationships between structure and properties, and models for structure generation. The subject is covered in sufficient depth to provide readers with the necessary background to understand the modeling techniques. The book will be of value to chemists in industries involved in the manufacture of organic chemicals such as solvents refrigerants, blood substitutes, etc. It also serves as a reference work for researchers, academics, consultants, and students interested in molecular design.

Prediction of Liquid-mixture Heat Capacity by Group Contribution Method

18th European Symposium on Computer Aided Process Engineering

A Group Contribution Method for Estimating Cetane and Octane Numbers

Vapor-Liquid Equilibria Using UNIFAC. A Group-Contribution Method. (Stichworte Teil 1)

Impact Evaluation in Practice, Second Edition

A comprehensive overview of current developments and applications in biofuels production Process Systems Engineering for Biofuels Development brings together the latest and most cutting-edge research on the production of biofuels. As the first book specifically devoted to process systems engineering for the production of biofuels, Process Systems Engineering for Biofuels Development covers theoretical, computational and experimental issues in biofuels process engineering. Written for researchers and postgraduate students working on biomass conversion and sustainable process design, as well as industrial practitioners and engineers involved in process design, modeling and optimization, this book is an indispensable guide to the newest developments in areas including: Enzyme-catalyzed

biodiesel production Process analysis of biodiesel production (including kinetic modeling, simulation and optimization) The use of ultrasonification in biodiesel production Thermochemical processes for biomass transformation to biofuels Production of alternative biofuels In addition to the comprehensive overview of the subject of biofuels found in the Introduction of the book, the authors of various chapters have provided extensive discussions of the production and separation of biofuels via novel applications and techniques.

Thermodynamic Modeling and Materials Data Engineering

Group-Contribution Method for Predicting Properties of Biochemical and Safety Interest and Temperature-Dependent Properties of Pure Components

Group Contribution Method for the Prediction of Glass Transition Temperatures of Amorphous Polymers

Development of an Improved Group Contribution Method for the Prediction of Vapour Pressures of Organic Compounds