Mass-Transfer Equation in Multicomponent Mixtures

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Abstract—A multicomponent mass-transfer equation for the distillation of multicomponent mixtures is derived in terms of the thermodynamics of irreversible processes.

It is well known that the notion of time is absent from classical thermodynamics. It usually considers equilibrium states or infinitesimal transitions from one equilibrium state into another. Meanwhile, real-world processes pass through nonequilibrium states, since they are driven by finite driving forces. The thermodynamics of processes far from equilibrium requires a quite complex mathematical apparatus [1].

In 1916, carrying out an experiment with a system containing hydrogen peroxide, formic acid, and sulfuric acid. Morgan observed a periodic generation of carbon monoxide. Somewhat later (1921), Bray detected that the H₂O₂ decomposition in an acidic medium in the presence of the iodate ion has an oscillatory character. In 1930, Frank-Kamenetskii proposed a theory of such oscillatory solutions. The mathematical formalism of these phenomena was borrowed from the Lotka-Volterra model of the periodic coexistence of predator and prev populations. In this model, the numbers of predator and prey individuals are described by nonlinear differential equations, which, as Poincare (1928) showed. have a totally different solution for oscillatory phenomena. Regardless of their initial state, such systems necessarily come to the same oscillatory motion, which is called the cycle [2].

The nonlinearity of differential equations is a necessary, but not sufficient, condition for oscillatory modes. This is because there are nonlinear processes that camnot occur in oscillatory modes. Among such processes are those whose linear approximation has a symmetric matrix of coefficients. The coefficients can be constants or certain functions of process variables. In the latter case, the symmetric matrix is a functional matrix. If a system is characterized by a nonsymmetric matrix A, it is necessary to determine whether or not this matrix is reduced to a symmetric matrix by the transformation [3]

 CAC^{-1} , (1)

where C and C^{-1} are a matrix and its inverse, respectively. The reduction to a symmetric matrix is possible if the real matrix A has characteristic roots.

Systems for which the first-approximation coefficient matrices are symmetric or can be reduced to symmetric are described in terms of the thermodynamics of linear irreversible processes, which has been sufficiently developed by Onsager and his school of thought. A more general case is the preservation of only the symmetry of the first-approximation coefficient matrices for a number of nonlinear systems. In this case, the first-approximation coefficients are functions of the state variables of the process under consideration [4, 5].

It was previously shown [6] that singular points of the set of paths of continuous distillation can only be generalized nodes or generalized saddles and cannot correspond to eigenvalues among which there are complex, conjugate, or imaginary numbers. Consequently, distillation can be described using the concepts of the thermodynamics of irreversible processes in generalized form.

There can be steady-state and unsteady-state distillation. An example of steady-state distillation is distillation in continuous columns. Examples of unsteadystate distillation are batch distillation and also the startup mode of continuous columns. The latter mode is conveniently represented in a configuration space with (n-1)(m'+2) or (n-1)(m'+1) ordinates, where n is the number of components, we is the number of plates in the rectifying section of a column, and m' is the number of plates in the stripping section of the column. In this case, unlike other representations, the state of the system is described by a point in the (n-1)(m+2)- or (n-1)(m'+1)-dimensional space and, depending on the initial state of the system, all unsteady-state processes are determined by the set of paths. Any of these paths ends at a singular point of the stable-node type. This is the point at which a given steady state takes place.

A system can have several steady states. For example, it can have two stationary points, one of which is an unstable node and the other is a stable node, or three

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Mass Transfer in Multicomponent Mixtures J. A. Wesselingh,2006 Multicomponent Mass Transfer Ross Taylor,R. Krishna,1993-12-16 Addresses the use of rigorous multicomponent mass transfer models for the simulation and design of process equipment Deals with the basic equations of diffusion in multicomponent systems Describes various models and estimations of rates of mass and energy transfer Covers applications of multicomponent mass transfer models to process design Includes appendices providing necessary mathematical background Contains a large number of numerical examples worked out in detail Modeling of Multicomponent Mass Transfer in Separation of Fluid Mixtures Eugeny Kenig,2000 Heat Transfer Equipment Design R. K. Shah, Eleswarapu Chinna Subbarao, R. A. Mashelkar, 1988-07-01

Two-Phase Flow Heat Exchangers Sadik Kakaç, Arthur E. Bergles, E. Oliveira Fernandes, 2012-12-06 Two phase flow heat exchangers are vital components of systems for power generation chemical processing and thermal environment control The art and science of the design of such heat exchangers have advanced considerably in recent years This is due to better understanding of the fundamentals of two phase flow and heat transfer in simple geometries greater appreciation of these processes in complex goemetries and enhanced predictive capability through use of complex computer codes The subject is clearly of great fundamental and practical importance The NATO ASIan Thermal Hydraulic Fundamentals and Design of Two Phase Flow Heat Exchangers was held in Povoa de Varzim near Porto Portugal July 6 17 1987 participating in the organization of the ASI were the Department of Mechanical Engineering and the Clean Energy Research Institute University of Miami Universidade do Porto and the Department of Mechanical Engineering Aeronautical Engineering and Mechanics Rensselaer Polytechnic Institute The ASI was arranged primarily as a high level teaching activity by experts representing both academic and industrial viewpoints The program included the presentation of invited lectures a limited number of related technical papers and discussion sessions Multicomponent and Multiscale Systems Juergen Geiser, 2015-08-21 This book examines the latest research results from combined multi component and multi scale explorations. It provides theory considers underlying numerical methods and presents brilliant computational experimentation Engineering computations featured in this monograph further offer particular interest to many researchers engineers and computational scientists working in frontier modeling and applications of multicomponent and multiscale problems Professor Geiser gives specific attention to the aspects of decomposing and splitting delicate structures and controlling decomposition and the rationale behind many important applications of multi component and multi scale analysis Multicomponent and Multiscale Systems Theory Methods and Applications in Engineering also considers the question of why iterative methods can be powerful and more appropriate for well balanced multiscale and multicomponent coupled nonlinear problems The book is ideal for engineers and scientists working in theoretical and applied areas Distillation Andrzej Gorak, Eva Sorensen, 2014-07-22 Distillation Fundamentals and Principles winner of the 2015 PROSE Award in Chemistry Physics is a single source of

authoritative information on all aspects of the theory and practice of modern distillation suitable for advanced students and professionals working in a laboratory industrial plants or a managerial capacity It addresses the most important and current research on industrial distillation including all steps in process design feasibility study modeling and experimental validation together with operation and control aspects This volume features an extra focus on the conceptual design of distillation Winner of the 2015 PROSE Award in Chemistry Physics from the Association of American Publishers Practical information on the newest development written by recognized experts Coverage of a huge range of laboratory and industrial distillation approaches Extensive references for each chapter facilitates further study The Use of High-purity Oxygen in the **Activated Sludge Process** J. R. McWhirter, 2019-07-30 First published in 1978 The purpose of this two volume series is to present a consolidated and comprehensive reference on oxygen activated sludge technology Fluid Transport in Nanoporous Materials Wm. Curtis Conner, Jacques Fraissard, 2006-03-10 This NATO ASI involved teachings and perspectives of the state of the art in experimental and theoretical understandings of transport in nanoporous solids This workshop brought together the top scientists and engineers in each area to discuss the similarities and differences in each technique and theory The lectures truly bridge the gaps between these related areas and approaches The applications in future separations catalysis the environment and energy needs are obvious The solids comprised the newly developing molecular sieves biological systems and polymeric solids Transport in single particles in membranes and in commercial applications were reviewed and analyzed placing each in context Techniques such as uptake Chromatographic Frequency Response NMR Neutron Scattering and Infrared spectroscopies are discussed for mixtures as well as for single components Theoretical approaches such as Density Functional Theory Statistical Mechanics Molecular Dynamics and Maxwell Stefan Theory are employed to analyze the diffusional transport in confined environments spanning from sub nanometers to centimetre scales In all cases the theories are related to the experiments These lectures present a unique opportunity to learn the various theoretical and experimental approaches to analyze and understand transport in nanoporous materials Chemical Engineering and Chemical Process Technology - Volume I Ryzhard Pohorecki, John Bridgwater, M. Molzahn. Rafigul Gani and Crispulo Gallegos, 2010-11-30 Chemical Engineering and Chemical Process Technology is a theme component of Encyclopedia of Chemical Sciences Engineering and Technology Resources in the global Encyclopedia of Life Support Systems EOLSS which is an integrated compendium of twenty Encyclopedias Chemical engineering is a branch of engineering dealing with processes in which materials undergo changes in their physical or chemical state These changes may concern size energy content composition and or other application properties Chemical engineering deals with many processes belonging to chemical industry or related industries petrochemical metallurgical food pharmaceutical fine chemicals coatings and colors renewable raw materials biotechnological etc and finds application in manufacturing of such products as acids alkalis salts fuels fertilizers crop protection agents ceramics glass paper colors dyestuffs plastics cosmetics

vitamins and many others It also plays significant role in environmental protection biotechnology nanotechnology energy production and sustainable economical development The Theme on Chemical Engineering and Chemical Process Technology deals in five volumes and covers several topics such as Fundamentals of Chemical Engineering Unit Operations Fluids Unit Operations Solids Chemical Reaction Engineering Process Development Modeling Optimization and Control Process Management The Future of Chemical Engineering Chemical Engineering Education Main Products which are then expanded into multiple subtopics each as a chapter These five volumes are aimed at the following five major target audiences University and College students Educators Professional practitioners Research personnel and Policy analysts managers and decision makers and NGOs Pervaporation, Vapour Permeation and Membrane Distillation Angelo Basile, Alberto Figoli, Mohamed Khayet, 2015-02-07 Vapour permeation and membrane distillation are two emerging membrane technologies for the production of vapour as permeate which in addition to well established pervaporation technology are of increasing interest to academia and industry As efficient separation and concentration processes they have high potential for use in the energy water chemical food and pharmaceutical sectors Part One begins by covering the fundamentals preparation and characterization of pervaporation before going on to outline the associated systems and applications State of the art uses future trends and next generation pervaporation are then discussed Part Two then explores the preparation characterization systems and applications of membranes for vapour permeation followed by modelling and the new generation of vapour permeation membranes Finally Part Three outlines the fundamentals of membrane distillation and its applications in integrated systems before the book concludes with a view of the next generation Explores three emerging membrane technologies that produce vapour as a permeate Looks at the fundamentals applications state of the art uses and next generation of each technology Provides an authoritative guide for chemical engineers and academic researchers interested in membrane technologies for desalination process water steam treatment water purification VOCs removal and other aspects of pollution control industrial process chemistry renewable energy production or separation and concentration in the food pharmaceutical industries Theoretical Foundations of Chemical Engineering ,1981 **Handbook of Phase** Change S.G. Kandlikar, 2019-01-22 Provides a comprehensive coverage of the basic phenomena It contains twenty five chapters which cover different aspects of boiling and condensation First the specific topic or phenomenon is described followed by a brief survey of previous work a phenomenological model based on current understanding and finally a set of Advances in Cryogenic Engineering K. Timmerhaus, 2013-11-21 The year 1973 marked the recommended design equa first time that Atlanta one of the cultural centers of the South has hosted the Cryogenic Engineering Conference since its beginning in 1954 The Cryogenic Engineering Conference gratefully acknowledges the hospital ity of the Georgia Institute of Technology and the assistance of W T Ziegler and his staff in making the visit to Atlanta a pleasant and memorable one Several significant changes were initiated at the 1973 Cryogenic Engineering Conference These included a Conference

theme on the subject of Energy and the Environment a new Conference format and the beginning of a new Conference frequency of biennial meetings While retaining the traditional topics of previous meetings the 1973 Cryogenic Engineering Conference focused on the role of cryo genic engineering in the generation distribution and conversion of energy and the related environmental effects In these areas much of the current interest stems from the environmental effects of LNG and liquid hydrogen as compared with other competing energy forms These rapidly expanding areas may provide the impetus to cryogenic engineering in the 1970 s that the space program provided in the 1960 s The Conference format was altered by the use of numerous invited papers highlighting the theme These presentations were concentrated in plenary sessions initiating each day's activities and in seminars designed to summarize the various aspects of the theme Nonequilibrium Thermodynamics Yasar Demirel, Vincent Gerbaud, 2025-02-17 This fully updated and revised fifth edition of Nonequilibrium Thermodynamics Transport and Rate Processes in Physical Chemical and Biological Systems emphasizes the unifying role of thermodynamics and their use in transport processes and chemical reactions in physical chemical and biological systems This reorganized new edition provides thermodynamical approaches for foundational understanding of natural phenomena with multiscale chemical physical and biological systems consisting of interactive processes leading to self organized dissipative structures fluctuations and instabilities This edition also emphasizes thermodynamic approaches tools and techniques including energy analysis process intensification and artificial intelligence for undertaking sustainable engineering This book will be an excellent resource for graduate students and researchers in the fields of engineering chemistry physics energy biotechnology and biology as well as those whose work involves understanding the evolution of nonequilibrium systems information theory stochastic processes and sustainable engineering This may also be useful to professionals working in irreversibility dissipative structures process exergy analysis and thermoeconomics digitalization in manufacturing and data processing Highlights the fundamentals of equilibrium thermodynamics and phase equilibria Expands the theory of nonequilibrium thermodynamics and its use in coupled reactions and transport processes in various time and space scales of physical chemical and biological systems Discusses self organized dissipative structures quantum thermodynamics information theory and stochastic approaches in thermodynamic analysis including fluctuation theories and molecular motors Includes new content on sustainable engineering with thermodynamics tools and techniques including energy analysis process intensification and artificial intelligencePresents many fully solved examples and numerous practice problemsOffers instructor resources containing a solution manual that can be obtained from the authors **Transport Processes Primer** Constantine Pozrikidis, 2019-11-08 In this concise yet comprehensive book the author discusses the principles of mass momentum and energy transport and derives balance equations for single component fluids and multicomponent mixtures based on the direct application of natural laws and principles of thermodynamics Transport equations over control volumes are formulated with reference to the Reynolds transport equation thereby circumventing the need for ad hoc balances for

open systems that are best justified in hindsight Notable features with regard to mass transport include the interpretation of diffusion in mixtures in terms of species parcel motion and separation the introduction of Fick's and fractional diffusion laws with reference to random molecular excursions a detailed account of species and mixture kinematics and dynamics and the discussion of partial stresses energies and entropies of individual mixture components Key features of this book include The governing equations are derived from first principles based on the application of natural laws and principles of thermodynamics Balances over control volumes are derived from rigorous equations governing material parcel property evolution Fick's law a fractional diffusion law and other diffusion laws are discussed with reference to random walks A detailed account of species and mixture kinematics and dynamics is presented for binary and multicomponent solutions A tabulated summary of transport equations is presented in differential and integral forms and an overview of classical thermodynamics is given in an appendix for a self contained discourse C Pozrikidis has taught at the University of California and the University of Massachusetts He is the author of several books on theoretical and computational topics in science and engineering applied mathematics scientific computing and computer science

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Principles and Modern Applications of Mass Transfer Operations Jaime Benitez, 2011-09-20 A problem solving approach that helps students master new material and put their knowledge into practice The Second Edition of the acclaimed Principles and Modern Applications of Mass Transfer Operations continues to provide a thorough accessible text that gives students the support and the tools they need to quickly move from theory to application This latest edition has been thoroughly revised and updated with new discussions of such developing topics as membrane separations ion exchange multistage batch distillation and chromatography and other adsorptive processes Moreover the Second Edition now covers mass transfer phenomena in biological systems making the text appropriate for students in biochemical engineering as well as chemical engineering Complementing the author's clear discussions are several features that help students guickly master new material and put their knowledge into practice including Twenty five to thirty problems at the end of each chapter that enable students to use their newfound knowledge to solve problems Examples and problems that help students become proficient working with Mathcad Figures and diagrams that illustrate and clarify complex concepts and processes References facilitating further in depth research into particular topics Ten appendices filled with helpful data and reference materials Ideal for a first course in mass transfer operations this text has proven to be invaluable to students in chemical and environmental engineering as well as researchers and university faculty **Fundamental Modeling of Membrane** Systems Patricia Luis, 2018-06-29 Fundamental Modelling of Membrane Systems Membrane and Process Performance summarizes the state of the art modeling approaches for all significant membrane processes from molecular transport to process level helping researchers and students who carry out experimental research save time and accurately interpret experimental data The book provides an overview of the different membrane technologies handling micro ultra and

nanofiltration reverse and forward osmosis pervaporation gas permeation supported liquid membranes membrane contactors membrane bioreactors and ion exchange membrane systems Examples of hybrid membrane systems are also included Presents an accessible reference on how to model membranes and membrane processes Provides a clear mathematical description of mass transfer in membrane systems Written by well known prominent authors in the field of membrane science *Collected Papers in Honor of Yoshihiro Shibata* Tohru Ozawa,2022-11-30 Yoshihiro Shibata has made many significant contributions to the area of mathematical fluid mechanics over the course of his illustrious career including landmark work on the Navier Stokes equations The papers collected here on the occasion of his 70th birthday are written by world renowned researchers and celebrate his decades of outstanding achievements

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