Horst Melcher and Ewald Gerth

Seven articles on reaction kinetics

in application to

atomic and nuclear physics, radiative transfer, oscillations, spectral line-profiles, pharmacokinetics

Keywords:
dynamic process, reaction system, reaction-space, radioactivity, nuclear conversion series, radiation transfer, absorption, Boltzmann's integro-differential equation, matrices, transformation, oscillations, coupling, line-profile-model, commutativity, time-reflection, impulse-behavior, pharmacokinetic reactions, bio-rhythms, frequency-pass, computer-programs

Collection of articles
printed as manuscripts
in Scientific Journals of the GDR
during the years 1970–1983

In 2014 published as monograph
by Herbert Utz Verlag GmbH, Munich, Germany
ISBN 978-3-8316-4403-2
www.utzverlag.de/catalog/book/44403

Editor: Dr. Ewald Gerth Potsdam 2014 Monograph

Preface

Seven publications on reaction kinetics, which came into being in the years from 1970 to 1983 in close cooperation of the authors Prof. Dr. Dr. Horst Melcher and Dr. Ewald Gerth, are put together in the present book with their thematical and methodical relations. The self-contained articles of this booklet are written in German. For English-speaking readers there are attached abstracts at the end of each article.

The seven articles contained in the present book represent only an exemplary selection from a wealth of processes, which determine all motions in nature and even in human society. The common theme of these publications is the description of the reaction course as a causal sequence of stochastic processes after Markov, represented analytically by matrices. The analogous transformation to other fields of application with a process-like character reveals a surprising multivalence of the method and opens new insights. The mathematical formulation of the reaction-kinetic process is given by the transformation of a vector, constituted by the components participating in the reaction system as a multidimensional vectorial space – the so-called "reaction space", and corresponds to a multiplication of the component vector with a resolving matrix. Any exchange of the sequence of processing periods yields different results, i.e., the exchange is non-commutative, which is an essential trait of all processes.

The publication of these treatises appeared at that time only in scientific journals within the restricted zone of the GDR. Therefore, it was decided by the authors to scan the printed originals and to restore the text in a monograph in order to make make it available to a wider circle of readers.

The edition of the book by E. Gerth was performed in agreement with Prof. Dr. Dr. Horst Melcher.

Ewald Gerth

Potsdam, June 2014

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(The seven abstracts and the epilogue are printed out on the following pages.)

Analytical treatment and numerical calculation of conversion series of radionuclides by means of matrix functions

Horst Melcher and Ewald Gerth

Abstract 1.

The analytical treatment of a process of radioactive reactions accompanied with conversion of chemical elements (spontaneous decay or build-up of the nucleus by capture of neutrons) can be afforded advantageously by formulating the system of linear differential equations by matrices, which yields at once an exact solution in its full entirety.

The solution is given by a matrix transformation of the nuclide components arranged as a vector of the nuclides, which is transformed in a "reaction space" by a resolving matrix during a transition process from an initial composition to the end composition.

The resolving matrix is represented as an expansion of a matrix exponential function, yielding immediately the algorithm for the numerical calculation in a computer program.

The linearity of the system of differential equations offers also the solution by using the Laplace-transformation, which is discussed concerning advantages and disadvantages compared to the expansion of the matrix exponential function (Neumann's row).

The application of vector algebra gives some interesting insight into the interconnection of the reacting components of the system: Thus, successive processes with different transition coefficients are commonly not commutative because of the non-commutativity of matrix-multiplication. The measured total radioactivity of the element composition is the scalar product of the column vector of nuclides and the row vector of detection probability. Every selected transition system is represented as a submatrix of the "global reaction matrix" comprising all possible nuclear transitions from hydrogen to transuranium.

Some numerical examples are given for the calculation of the uranium row and the conversion of gold to mercury.

Treatment of radiative transfer by means of matrix functions

Horst Melcher and Ewald Gerth

Abstract 2.

The transport equation of Boltzmann is formulated and solved by means of an infinite equation of matrices for the case of the stationary rectilinear propagation of radiation with respect to energy scattering only. It is shown that the matrix formalism is the proper one to explain the qualities of transformations and the non-commutativity of the radiation transmitted through compound, heterogeneous layers of material.

The resolving matrix is represented as an expansion of a matrix exponential function, yielding at once the algorithm for the numerical calculation in a computer program. The linearity of the system of differential equations also offers the solution by using the Laplace-transformation, which reveals the structure of the resolving matrix compared to the expansion of the matrix exponential function.

The matrix formalism renders a comprehensive method for analytical derivation, numerical computation, and definition of relations among different interacting physical magnitudes. Thus, using the matrix calculus, a new definition for the average length of reach of the radiative transfer through an absorbing medium could be given in form of the inverse kernel matrix of the transport equation.

Solution of the stationary radiation transport problem for energy scattering using matrix functions

Horst Melcher and Ewald Gerth

Abstract 3.

The radiation transport equation of Boltzmann is formulated and solved by means of an infinite equation of matrices for the case of stationary rectilinear propagation of radiation with respect to energy scattering only.

It is shown that the matrix formalism is the proper one to explain the qualities of transformations and the non-commutativity of the radiation transmitted through compound, heterogeneous layers of material.

Furthermore, an analytical and perspicuous representation of the transmission of divergent beams is given.

Finally, simple equations for the flux of radiation, the mean range, and the counting rate are set up.

Oscillations represented as a transformation problem of matrix functions

Horst Melcher and Ewald Gerth

Abstract 4.

Oscillations are usually represented as the solution of a differential equation of the second order. From this conventional form of the solution, it is not evident at immediately that the oscillating system goes over from a state at the beginning to a state at a later time by transformation of the components.

In the article referred to here, it is demonstrated that oscillations can definitely be characterized as a problem of transformation by means of matrices which reproduces completely the classical solution to the oscillation differential equation. The oscillation is regarded as a reaction process, which is simulated in a functional sequence of small steps establishing the resolving matrix by expansion of a matrix exponential series. There is no need for the solution to any eigenvalue problem.

The application of matrices, moreover, proves to be especially suitable for the analytical treatment and numerical calculation of coupled oscillators. Coupling is investigated by the resonance of an oscillator on excitation of external oscillations. By this means, one can describe even extended systems of coupled oscillators like atoms and molecules in a crystal lattice in different mutual relations and spatial arrangements.

The matrix version of treatise oscillation processes offers the advantage that it can be adjusted to the well-developed methods of the solution to interacting reaction systems, the calculating algorithms of which are already available. In such a reaction system an oscillator is represented as a reacting component by a two-row elementary submatrix of the type of Pauli's spin matrices. Thus, also the combination with other – e.g., physical, chemical, or biological – reaction systems and the simultaneous solution of them is possible.

A heuristic model for spectral-line-profiles

Horst Melcher and Ewald Gerth

Abstract 5.

By means of the Fourier-transformation for the statistical Poisson-distribution a function $y(x)$ is obtained, which is called in this paper the Lorentz-function of n-th degree:

$$y = (1 + x^2)^{-n}.$$

Special cases such as $n = 1$ or $n \to \infty$ are used for representing types of spectral lines: the Lorentz- or dispersion-type and the Gauss-type, resp. Up to now the region between these two types has been represented by the so-called Voigt-function. The new general Lorentz-function is suitable for approximating or replacing the complicated Voigt-function.

The general Lorentz-function is based upon an abstract model which is valid for processes in kinetic systems or in electronic networks.

Representation of spectral line profiles by means of the Lorentz-function of n-th degree

Horst Melcher and Ewald Gerth

Abstract 6.

It will be shown how to fit the Lorentz-function of n-th degree to profiles of the spectral lines. Some examples are given for analyzing profiles by a new method, called the "cutting-method". Values of the Voigt-function are compared with those of the general Lorentz-function (of n-th degree). It seems to be impossible to differentiate these two functions by means of experimental methods. The results of the analysis of profiles yielding $n < 1$ may be due to those profiles being composed of two or more components.

Commutativity, time-reflection, and impulse-behavior of pharmacokinetic reactions

Horst Melcher and Ewald Gerth

Abstract 7.

In continuation of former works of the authors in other fields of physics, it is shown that the matrix-calculation can be applied profitably also to problems in the field of pharmacology. That refers above all to the concepts of commutativity and non-commutativity as well as to the impulse-behavior by administering different pharmacological drugs.

The main focus of the present work is concentrated on the analytic representation of reaction systems and reaction processes. An appropriate analytical formulation and treatment of kinetic reaction processes is given by the matrix-calculation which implies the extremely important **non-commutativity** of the multiplication of matrices. The reaction process is pursued in positive time-progression and in negative direction of time by **time-reflection**. The relevant differential equation systems are formulated as vector-transformations of the "concentration-vector" in the multidimensional "reaction-space".

The reaction-matrix is considered also for temporally variable transition coefficients. With the reference to such phenomena like the propagating and spreading of concentration impulses in the reaction medium, also oscillating reactions are represented as effects brought about by intermittently given pharmacological drugs, showing a characteristic **impulse-behavior**. Thus, biorhythms, periodical seasons of the year and the day, with averaging, resonance, and aftereffect can be described analytically and, using special computer programs for the solution of nonlinear systems of differential equations, can be calculated numerically.

Epilogue

The *Seven Articles on Reaction-kinetics* are a testimony of an enduring prolific scientific cooperation. They reflect, however, the level of knowledge of half a century ago and should be actualized – concerning as well the contents as the referred literature. After the presentation of the original articles in the internet and the approval to print by the *Herbert Utz Verlag*, the authors Prof. Dr. Dr. H. Melcher and Dr. E. Gerth considered a reworking of the material. Due to advanced age, however, the authors decided on a "moderate solution".

To this end, it was proposed by E. Gerth to perform a soft reworking together with text processing and wrapping, whereby the basic character of the articles would be preserved. Above all there should be new examples of computation with graphic representations. Fifty years ago one still was used to programming with the first suitable calculation machines, further then computing, punching on paper tapes, storing intermediately, printing on a typewriter, evaluating and – after all – drawing on paper by hand. In this way the first article of this book on radioactive conversion series was made.

After the publication of the seven articles in scientific journals of the GDR, also in computing techniques a change occurred. Now, personal computers were available for everybody, which enabled one to work independently of official computer centers. By means of the development of a computer program for the implicit integration of systems of nonlinear differential equations and computer graphic, it became possible to prove the different reaction systems in a rapid course of computation and to represent the results clearly arranged on a screen as well as to make patterns of them suitable for printing.

Regardless of the possibility to now outfit out all articles of the book with diagrams, we consider the matter closed here. Merely the article on oscillations in matrix representation, which at that time was left as a "fragment" for lack of computing capacity, has been amplified by several sections, making illustrative the coupled oscillations by diagrams obtained by computer calculation.

Reaction processes are omnipresent. Many questions arising from this book remain open. In any case, the book may stimulate the interested reader to a further application of the matrix-method for the calculation of processes!

Potsdam, June 2014 *Ewald Gerth*