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# Mathematical Methods, Computational Techniques, Intelligent Systems

**12<sup>th</sup> WSEAS International Conference on Mathematical Methods,  
Computational Techniques and Intelligent Systems (MAMECTIS '10)**

**Kantaoui, Sousse, Tunisia, May 3-6, 2010**

**Sponsor and Organizer:**

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**Mathematics and Computers in Science and Engineering  
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**ISBN: 978-960-474-188-5**

**ISSN: 1790-2769**

**Published by WSEAS Press**

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All papers of the present volume were peer reviewed by two independent reviewers. Acceptance was granted when both reviewers' recommendations were positive.  
See also: <http://www.worldses.org/review/index.html>

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**Preface**

This year the 6th WSEAS International Conference on 12th WSEAS International Conference on MATHEMATICAL METHODS, COMPUTATIONAL TECHNIQUES AND INTELLIGENT SYSTEMS (MAMECTIS '10) was held in Kantaoui, Sousse, Tunisia, May 3-6, 2010. The conference remains faithful to its original idea of providing a platform to discuss new intelligent systems, new mathematical methods, new computational techniques or applications of known mathematical methods and computational techniques, finite differences, finite volumes, variational calculus, stochastic systems, cellular automata, universal approximants, evolutionary computing, electronics, microelectronics, nanoelectronics power systems automation, control, robotics electromagnetic fields fluid mechanics quantum mechanics etc. with participants from all over the world, both from academia and from industry.

Its success is reflected in the papers received, with participants coming from several countries, allowing a real multinational multicultural exchange of experiences and ideas.

The accepted papers of this conference are published in this Book that will be indexed by ISI. Please, check it: [www.worldses.org/indexes](http://www.worldses.org/indexes) as well as in the CD-ROM Proceedings. They will be also available in the E-Library of the WSEAS. The best papers will be also promoted in many Journals for further evaluation.

A Conference such as this can only succeed as a team effort, so the Editors want to thank the International Scientific Committee and the Reviewers for their excellent work in reviewing the papers as well as their invaluable input and advice.

The Editors



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## Plenary Lecture 1

### Dynamical Calculations on Hydrogen-oriented Chemical Reactions



**Professor Wensheng Bian**

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**Abstract:** The hydrogen transfer, abstraction and exchange reactions for hydrogen-rich compounds are of considerable importance in environmental and hydrogen energy chemistry. Interest in acetylene–vinylidene isomerization is long-standing,<sup>1-3</sup> which is a benchmark for the study of hydrogen migration. The lifetime of vinylidene was long accepted as being very short, however, in 1998, a very long lifetime of at least 3.5 microseconds was claimed.<sup>2</sup> We report the first full-dimensional quantum-mechanical calculations on the isomerization of acetylene to vinylidene on an ab initio potential energy surface. Our theoretical scheme is a combination of several methods. The Jacobi coordinates are chosen and a kind of complex absorbing potential is used to deal with the isomerization behaviour of vinylidene, which is made possible by a novel reaction coordinate defined by us. Phase space optimization in combination with physical considerations<sup>3</sup> is used to obtain an efficient radial discrete variable representation, whereas a basis contraction scheme is applied for angular coordinates; The preconditioned inexact spectral transform method combined with an efficient preconditioner is employed to compute complex eigenstates within a desired spectral window. Our computation is very efficient, and the computed state-specific lifetimes of vinylidene will be reported and discussed in terms of experimental divergences and isomerization mechanism. The abstraction reaction of  $\text{H}+\text{SiH}_4$  plays a significant role in chemical vapor deposition processes used in semiconductor industry, and the competition between hydrogen abstraction and exchange in this system is typical. We constructed an accurate global 12-dimensional ab initio potential energy surface,<sup>4</sup> which describes both the  $\text{H}+\text{SiH}_4$  abstraction and exchange reactions, and performed further dynamical calculations. Our QCT calculations reveal interesting features of detailed dynamical quantities and underlying new reaction mechanisms. We designate new mechanisms for exchange found by us as torsion-tilt and side-inversion. The abstraction reaction is shown to be a combination of rebound and stripping. Results and findings from our recent dynamical studies will be reported, which are important for acquiring a deeper understanding of polyatomic abstraction and exchange reactions.

## Plenary Lecture 2

### **Identities and Inequalities Derived from Euclid's Algorithm with Applications in Cutting-Covering Receipts**



#### **Professor Marius Paun**

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**Abstract:** Starting from the original demonstration of the Euclid's Algorithm (Elements, Book VII,2) we deduce one using rectangles. From this proof we deduce after some calculus some identities and inequalities that we use in Cutting-Covering Receipts.

#### **Brief Biography of the Speaker:**

Dr. Paun Maris is an Associate Professor at the department of ALGEBRA, GEOMETRY AND DIFFERENTIAL EQUATIONS in the Faculty of Mathematics and Informatics, Transilvania University of Brasov, Romania. He is a Ph.D in Applied Mathematics and his field of expertise is Invariant frames in Lagrange spaces. Author of more than 40 articles on this subject or connected ones published in BDI Journals or proceedings of international conferences. Member of The Balkan Society of Geometers and censor of this scientific society. His teachable span the fields of Algebra, Special mathematics and Differentiable Geometry. Deputy chair of the department he works in.

## Plenary Lecture 3

### Mathematical Models of Dusty Gas Flow through Porous Media



**Professor M. H. Hamdan**

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**Abstract:** This work reports on the recent advances in the continuum approach to dusty gas flow modeling through isotropic porous structures. This approach has received considerable attention over the last half century due to the need to develop dusty gas flow models capable of describing natural and industrial transport phenomena, including the subsurface transport of dissolved or suspended particulates, the design of liquid-dust separators, and the analysis and design of filtration systems.

A number of models have recently been developed to describe gas particulate flow through porous media, and account for both the macroscopic flow behavior as well as the microscopic interactions that arise due to the porous microstructure. Detailed knowledge of porous microstructures leads to a better understanding of the interactions between the phases involved, and of the forces exerted by the porous matrix on the flowing phases. Mathematical idealization of porous microstructures has been implemented in the developed models, which describe various dusty gas flow situations and particle transport through porous structures.

We discuss in this work models that assume either a uniform or variable distribution of particles in the flow field, and models that provide for modeling flexibility using phase partial pressures. Appropriate boundary conditions associated with the above models are also analyzed.

**Brief Biography of the Speaker:**

M. H. Hamdan received an Ordinary National Diploma in Technology-Engineering from Swindon College, U.K.; a Certificate in Negotiation, Mediation and Conflict Resolution from St. Mary's University, Canada; a B.Sc, M.Sc., and a Ph.D in Applied Mathematics from the University of Windsor, Canada. He taught at a number of universities both as a regular faculty member and as a visiting professor, in Canada, China and the Middle East. He has been teaching at the University of New Brunswick, Canada, for 19 years, and is a previous Chair of the Department of Mathematics, Statistics and Computer Science. His teachables span the areas Mathematics, Decision Sciences and Management Science, Mathematical Economics, and Negotiations. His research areas include computational fluid dynamics, single-phase flow through porous media, and modeling dusty gas flow through porous media. He is an International Consultant in Science and Technology Planning and in School Mathematics Curricular Development. He is the recipient of a number of teaching awards, and is listed among American Men and Women of Science; Who's Who in Science and Engineering; Who's Who in the World; and Two Thousand Outstanding Scientists of the 20th Century.