



Editors

Jose Alberto Duarte Moller

Maurice R. Kibler

Ray Hefferlin



Recent Advances in Chemical Engineering, Biochemistry and Computational Chemistry

- ✦ Proceedings of the 4th WSEAS International Conference on Biochemistry and Medical Chemistry (BIOMEDCH '13)
- ✦ Proceedings of the 7th WSEAS International Conference on Computational Chemistry (COMPUCHEM '13)
- ✦ Proceedings of the 4th European Conference of Chemical Engineering (ECCE '13)

Paris, France, October 29-31, 2013

Scientific Sponsors



ISBN: 978-960-474-342-1



RECENT ADVANCES in CHEMICAL ENGINEERING, BIOCHEMISTRY and COMPUTATIONAL CHEMISTRY

**Proceedings of the 4th WSEAS International Conference on Biochemistry and
Medical Chemistry (BIOMEDCH '13)**

**Proceedings of the 7th WSEAS International Conference on Computational
Chemistry (COMPUCHEM '13)**

**Proceedings of the 4th European Conference of Chemical Engineering
(ECCE '13)**

**Paris, France
October 29-31, 2013**

Scientific Sponsors:



University of Zagreb, Croatia



European Institute of Informatics and
Educational Technology in Belgrade, Serbia



Music Academy "Studio
Musica", Italy



Constanta Maritime
University, Romania



Ain Shams University,
Egypt

RECENT ADVANCES in CHEMICAL ENGINEERING, BIOCHEMISTRY and COMPUTATIONAL CHEMISTRY

**Proceedings of the 4th WSEAS International Conference on Biochemistry and
Medical Chemistry (BIOMEDCH '13)**

**Proceedings of the 7th WSEAS International Conference on Computational
Chemistry (COMPUCHEM '13)**

**Proceedings of the 4th European Conference of Chemical Engineering
(ECCE '13)**

**Paris, France
October 29-31, 2013**

Published by WSEAS Press

www.wseas.org

Copyright © 2013, by WSEAS Press

All the copyright of the present book belongs to the World Scientific and Engineering Academy and Society Press. All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior written permission of the Editor of World Scientific and Engineering Academy and Society Press.

All papers of the present volume were peer reviewed by no less than two independent reviewers. Acceptance was granted when both reviewers' recommendations were positive.
See also: <http://www.worldses.org/review/index.html>

ISBN: 978-960-474-342-1

RECENT ADVANCES in CHEMICAL ENGINEERING, BIOCHEMISTRY and COMPUTATIONAL CHEMISTRY

**Proceedings of the 4th WSEAS International Conference on Biochemistry and
Medical Chemistry (BIOMEDCH '13)**

**Proceedings of the 7th WSEAS International Conference on Computational
Chemistry (COMPUCHEM '13)**

**Proceedings of the 4th European Conference of Chemical Engineering
(ECCE '13)**

**Paris, France
October 29-31, 2013**

Editors:

Prof. Jose Alberto Duarte Moller, Centro de Investigación en Materiales Avanzados, Mexico

Prof. Maurice R. Kibler, Université de Lyon, France

Prof. Ray Hefferlin, Southern Adventist University, TN, USA

Committee Members-Reviewers:

Jean-Michel Jault

Hassane Oudadesse

Anita H. Corbett

Toshiharu Horie

Vadim V. Sumbayev

Andre Surguchov

Rona R. Ramsay

Daniel Martins-de-Souza

Roberta Chiaraluce

George Perry

David Brown

Gertz I. Likhtenshtein

Ziad Fajloun

Vivo Turk

Makoto Komiyama

Hundie Tesfaye

Shunsuke Meshitsuka

George A. Zachariadis

K. Balasubramanian

Benoit Champagne

Markus Meuwly

M. Nakano

Ajit J. Thakkar

B. Akay

J. Czernek

H. Kao

A. Mohajeri

R. Singh

K. Ruud

H. Torii

S. Consta

K. Harigaya

M. Riad Manaa

Paul M. Lahti

Michael J. Bucknum

Eduardo A. Castro

Sourav Pal

N. A. Besley

F. Jensen

T. A. Wesolowski

P. Cortona

Zhibing Zhang

Adrian Schumpe

Jerzy Baldyga

Alirio Rodrigues

Mostafa Barigou

Jaime Wisniak

Sohail Murad

Konstantinos E. Kakosimos

Raghunath V. Chaudhari

Xijun Hu

Deepak Kunzru

Lucija Foglar

John Antonopoulos

Al Emran Ismail

Alina Adriana Minea

Liana Anica-Popa

Matteo Palai

Zahéra Mekkioui

Csaki Apostolescu Ioana

Emadoddin Abbasi

Francisc Popescu

Libor Pekar

Tomas Ganiron Jr

Table of Contents

Plenary Lecture 1: Nanoparticles as Targeting Delivery Vehicles for Brain Disease Treatment	9
<i>Yung-Chih Kuo</i>	
A New Multiresolution Model for Catalytic Converter Systems	11
<i>Cansu Ozhan, Daniel Fuster, Patrick Da Costa</i>	
Simulating the Transient Regimes and Concentrate Waves in Through-Reactors with Multi-Stage Kinetics	18
<i>M. Yunussov, A. Kalbayeva, S. Kurakbayeva, A. Brener</i>	
Sugars Production from Wheat Straw Using Maleic Acid	23
<i>G. Katsamas, D. Sidiras</i>	
Effect of pH on Physical Properties of Edible Films from Faba Bean Protein	29
<i>C. Montalvo-Paquini, M. Rangel-Marrón, E. Palou, A. López-Malo</i>	
Nanocomposites of Ethylene Vinyl Acetate Copolymer and Clay	35
<i>Dagmar Merinska, Alena Kalendova, Zuzana Dujkova, Miroslav Slouf, Josef Simonik</i>	
Enzymes in Biotransformation	41
<i>Jelenka Savkovic-Stevanovic, Jelena Djurovic, Milena Stevanovic-Huffman</i>	
Distribution and Risk Assessment of Polychlorinated Biphenyls (PCBs) in Urban Soils of Sofia City, Bulgaria	48
<i>Anna Dimitrova, Yana Stoyanova, Anton Tachev</i>	
PE and PP Clay Nanocomposites - Structure Modeling and Properties	55
<i>D. Merinska, A. Kalendova, M. Pospisil</i>	
Oxygen Transfer in the Blood	60
<i>Jelenka Savkovic-Stevanovic</i>	
Determination of Transport Characteristics of Porous Biocompatible Materials	66
<i>Karel Soukup, Vladimír Hejtmánek, Olga Šolcová</i>	
Optimization of the Moisture Content, Thickness, Water Solubility and Water Vapor Permeability of Sodium Alginate Edible Films	72
<i>M. Rangel-Marrón, C. Montalvo-Paquini, E. Palou, A. López-Malo</i>	
Multi-Core Programming for Bio-Reaction Mining Model of Eugenol-Induced Apoptosis with Honey for Cancer Treatment	79
<i>Chandrasekaran Subramaniam, Manasa Priyamvada, Sriram Suruliandi</i>	
Multiscale Convergence Optimization in Constrained Molecular Dynamics Simulations	84
<i>N. M. Nafati, S. Antonczak, J. Topin, J. Golebiowski</i>	

Thermal Conductivity of Organic Liquids: A New Equation	91
<i>Di Nicola Giovanni, Ciarrocchi Eleonora, Pierantozzi Mariano, Stryjek Roman</i>	
Authors Index	96

Plenary Lecture 1

Nanoparticles as Targeting Delivery Vehicles for Brain Disease Treatment



Professor Yung-Chih Kuo
Department of Chemical Engineering
National Chung Cheng University
Chia-Yi, Taiwan, Republic of China
E-mail: chmyck@ccu.edu.tw

Abstract: Finely controlled formulations of nanoparticulate excipient to carry pharmaceuticals and regimens into the central nervous system (CNS) are emerging challenges to the therapy for diseases and neurological disorders in clinical practice. This speech shows the nanoparticle drug delivery systems for medicinal applications. We will discuss the characteristics of colloidal carriers, including the particle size distribution, particle exterior geometry and interior structure, surface charge density, and targeting molecules on particle surface. These physicochemical and biological properties are the most crucial factors affecting the colloidal behavior in biomedical technology. In addition, the efficacy of various nanocarriers in treating brain pathology will be evaluated. Acute ischemic stroke, brain tumor, Alzheimer's disease, and Parkinson's disease are among the highlighted pathological issues using the nanoparticulate system in the current stage. Moreover, the targeting transport of functionalized nanoparticles across the blood–brain barrier will be addressed. Nano-structured colloids can be promising and competent biomaterials for delivering drugs into the brain and producing curative effects on thorny CNS diseases.

Brief Biography of the Speaker: Dr. Yung-Chih Kuo is a professor at the Department of Chemical Engineering, National Chung Cheng University. His research interests are focused on biomaterials, drug delivery system, tissue engineering, blood–brain barrier, stem cell differentiation, nerve regeneration, cancer therapy, Alzheimer's disease treatment, biophysics, and colloid and interface science. In these fields, he has authored or coauthored over 120 SCI journal papers. He is an honor member of Phi Tau Phi Society, a life member in various academic Societies including American Nano Society, European Atherosclerosis Society, Asia-Pacific Chemical, Biological and Environmental Engineering Society, Asian Federation of Biotechnology, Asian Biotechnology Directory, Taiwanese Society of Biomedical Engineering, Chinese Institute of Engineers, Taiwan Institute of Chemical Engineers, Biochemical Engineering Society of Taiwan, and Taiwan Biomaterials and Controlled Release Society. He won Young Scholar Award in 2003 and Distinguished Research Award in 2011 and 2013. He is also an associate editor of J. Taiwan Inst. Chem. Engrs. (Impact factor 2.110) and an editorial board member in 6 international journals, and has been invited as a manuscript reviewer for over 50 journals (top reviewer of the Journal of Physical Chemistry (American Chemical Society)), an external reviewer for European research proposals, academic awards, research grants, faculty recruitments and promotions, and financial support of hosting international symposiums, and an advisory board committeeman of international conferences and symposiums.

Authors Index

Antonczak, S.	84	Palou, E.	29, 72
Brener, A.	18	Pierantozzi, M.	91
Ciarrocchi, E.	91	Pospisil, M.	55
Da Costa, P.	11	Priyamvada, M.	79
Di Nicola, G.	91	Rangel-Marrón, M.	29, 72
Dimitrova, A.	48	Savkovic-Stevanovic, J.	41, 60
Djurovic, J.	41	Sidiras, D.	23
Dujkova, Z.	35	Simonik, J.	35
Fuster, D.	11	Slouf, M.	35
Golebiowski, J.	84	Šolcová, O.	66
Hejtmánek, V.	66	Soukup, K.	66
Kalbayeva, A.	18	Stevanovic-Huffman, M.	41
Kalendova, A.	35, 55	Stoyanova, Y.	48
Katsamas, G.	23	Stryjek, R.	91
Kurakbayeva, S.	18	Subramaniam, C.	79
López-Malo, A.	29, 72	Suruliandi, S.	79
Merinska, D.	35, 55	Tachev, A.	48
Montalvo-Paquini, C.	29, 72	Topin, J.	84
Nafati, N. M.	84	Yunussov, M.	18
Ozhan, C.	11		