Prof. Dr. Ing. Gheorghe MARIA

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https://new.acad.ro/acad_membri/

I. SCIENTIFIC PROFILE

PERSONAL DATA

Date and place of birth: Gheorghe MARIA (GM) was born on October 2, 1955, in the village Fundeni, Călăraşi county, Romania.

EDUCATION

- Primary school (gymnasium) in Bucharest (1962-1970).
- Graduate of the high school "Gh. Lazăr" from Bucharest (1970-1974) - special class of mathematics and chemistry (**science** profile).
- During high school, he participated to numerous national competitions (Olympics) in Chemistry and Mathematics, winning several prizes. In 1974, he participated to the 6th International Chemistry Olympiad for high school students [1-2]. At this famous competition with a long tradition (11 participating countries: Russia, Eastern European countries, Germany, Sweden, Austria, etc.), GM won the gold medal (**Fig. 1A**) by presenting ingenious mathematical solutions to difficult chemical problems. Impressed by his success, the writer E. Seceleanu dedicated a chapter to him in his book [3].

- Graduate of the Faculty of Chemical Technology (formerly known as Faculty of Industrial Chemistry) of the Polytechnic University of Bucharest (**U.P.Buc.**) (formerly the Polytechnic Institute of Bucharest). At U.P.Buc. he followed 5-year studies (bachelor's and master's) in the specializations of Organic Chemistry and Chemical Engineering. Graduate in 1979 as Valedictorian (Chemical Engineer degree) (**Fig. 2A**).
- Supervisor of the bachelor thesis (engineer diploma): late Prof. Dr. Eng. Octavian Smigelschi. Title of his diss.: "Mathematical Modeling and Optimization by using advanced Numerical Algorithms of a Multi-partitioned Sugar Extractor"(1979) (**Fig. 2A**).
- The supervisor of his MSc. Diss. in Chemical and Biochemical Engineering (**ICB**): late Prof. Dr. Eng. Raul Mihail. Dissertation title: "Mathematical modeling and numerical simulation of the tubular reactor used for the hydrocarbon pyrolysis, and of the radiative heat transfer in the pyrolysis furnaces" (1979) (**Fig. 2A, Fig. 9**).
- Numerous research grants and temporary positions at prestigious universities abroad (see below, in chronological order).

SCIENTIFIC TITLES

- 1987 (June). PhD in Chemical Engineering at **U.P.Buc.**, under the supervision of the late Prof. Dr. Eng. Raul Mihail, with the thesis: "The Statistical Estimation of the Parameters of Mathematical Models of Chemical and Biochemical Processes" (**Fig. 2A**).
- 2019 (30 May). Elected (by unanimous vote) as Corresponding Member of the Romanian Academy (Chemical Sciences section) (**Fig.3**). **https://new.acad.ro/acad_membri/membri/Maria_Gheorghe.html**
- 2020 (January). President of the Chemical and Biochemical Engineering Commission (**ICB**) of the Romanian Academy (Chemical Sciences section) (**Fig.16**).
- 1985. "Nicolae Teclu" Award of the Romanian Academy (**Fig. 6**).

JOBS HELD (CAREER)

Dr. G. Maria (**GM**) has had an exceptional career as a chemical engineer, spanning over more than four decades, by accumulating experience from **all sides of his profession**: production, research, industrial plant design, and high education, **holding positions** and carrying out numerous research internships abroad at prestigious universities in EU, USA, and China within international research projects. Among them, the following should be mentioned:

1979-1982: internship (mandatory) in chemical industry, as a plant engineer at chemical enterprises in Bucharest ("Miraj" and "Chimica" Dudești);

1982-1990: (by open competition) senior researcher at ICECHIM – The Chemical and Biochemical Energetics Institute of Bucharest (**IECB**), in-charge with the mathematical modeling of catalytic and (bio)chemical processes kinetics, and with the technological design of chemical catalytic plants at various scales (including the industrial one);

1990: (by open competition) he became lecturer at **U.P.Buc.**, Dept. of Chemical Engineering, Lab. Of Reactors and Chemical and Biochemical Reaction Engineering (**Fig. 2B**);

1992-1997: Following an invitation, he came in Switzerland, being hired as Assistant Professor (Oberassistent Klass 18) at the Polytechnic Institute ETH Zürich (Switzerland), Dept. of Chemical Engineering (Technische Chemie), the "Process Systems Engineering" group of the late Prof. Dr. Eng. D.W.T. Rippin, being in-charge with teaching and research duties in Chemical and Biochemical Engineering, as well as Chemical Process Risk Analysis.

1997: (by open competition) he became assoc. professor with **U.P.Buc.**, Dept. of Chemical Engineering (**ICB**), Lab. Reactors, and of Chemical and Biochemical Reaction Engineering [4].

1999: (by open competition) he became habil. Professor at **U.P.Buc.**, Dept. of Chemical and Biochemical Engineering (**ICB**), Lab. Reactors, and of Chemical and Biochemical Reaction Engineering [4];

2008: habil. professor supervisor of PhD-s at UPBuc., department of Chemical and Biochemical Engineering, Lab. Reactors, and Chemical and Biochemical Reaction Engineering [4];

2014: A severe stroke caused the cancellation of all foreign travels. However, Prof. GM managed to continue on-line some scientific collaborations.

2020: (retirement) retired university professor. He continue to supervise PhD-s at **U.P.Buc.**, Dept. of Chemical and Biochemical Engineering, Lab. (Bio)Chemical Reactors. He continue his research activity also in the framework of the Romanian Academy.

RESEARCH INTERNSHIPS, SCHOLARSHIPS, TEMPORARY POSITIONS ABROAD

- **1992-1996**. Asistant Professor (Oberassistent Klass 18) at Swiss Federal Institute of Technology - **ETH Zürich** (Switzerland), Dept. of Chemical Engineering (Technische Chemie), "Systems Engineering Group" of late Prof. David W.T. Rippin (1992-1995), and then in the group of „Non-conventional Sources of Energy" led by Prof. Alexander Wokaun (1996)(**Fig.7**);
- **1997** (Aug-Oct). Research internship at **ETH Zürich** (Switzerland), Dept. of Chemical Engineering, as director / key researcher in the SNSF (Swiss National Science Foundation) project no. 7IP - 050113/1997-1998: „Ecological and Risk Analysis in Chemistry" (group of Prof. E. Heinzle; dr. A. Keller –Roche, Basel);
- **1999** (July-Aug). Visiting Professor within DAAD Research Grant no. 324-ro-99/1999 at Universität des **Saarlandes** (Germany), Dept. Of Biochemical Engineering, with the theme: „Testing Novel Short-Cut Methods for Kinetic Characterisation of Biochemical Processes" (Prof. Elmar Heinzle);
- **2000** (Feb-March, Nov-Dec). Guest Professor at University of **Porto** (Portugal), Departamento de Engenharia Quimica (Automatics & Robotics in Bio-Chemistry), Director of NATO Grant no. 974850-99/1999-2001 „Identification of Optimal Operating Conditions and Risk Limits for Biological Wastewater Treatment Plants" (group of Prof. Sebastiao Feyo de Azevedo, and Prof. Romualdo Salcedo);
- **2000** (June-Aug). Guest Professor at Technische Universität **Erlangen-Nürnberg** (Germany), Dept. of Chemical Eng. Key researcher in the project: „Kinetics Identification and Process Simulation for the Drinking Water Denitrification via a Three-Phase Catalytic Membrane Reactor" (group of late Prof. G. Emig and of Prof. Roland Dittmeyer);
- **2002 – 2003**. Research Scientist / invited professor at **Texas A&M University** (College Station, Texas, USA), Dept. of Chemistry and Cellular Biology, with a scholarship from the National Institute of Health (NIH) for the NIH project no. PAL-GM63958/2002-2003, with the theme: „Kinetic simulations of minimal living systems", and for the NIH project no. EES-GM64650/2002-2003, with the theme: „Molecular recognition in dendrimers based on melamine - Kinetics of programmable drug release in human plasma", (Prof. E. Simanek and prof. P. Lindahl);
- **2006** (July). Guest Professor at Technische Universität **Braunschweig** (Germany), and at German Research Centre for Biotechnology, as part of DFG-578 project, with the theme: „Development of Biotechnological Processes by Integrating Genetic and Engineering Methods" (late Prof. Wolf Deckwer);
- **2009** (July-August). Visiting Professor within DAAD Research Grant no. A/09/02572/2009, with the theme: „Dynamic modelling of some genetic regulatory circuits to simulate the bacterial resistance in a polluted environment by using the whole-cell modelling approach", at Technische Universität **Hamburg** (TUHH), Institute of Bioprocess & Biosystems Engineering (Germany) (group of Prof. An-Ping Zeng);
- **2010** (July-August). Visiting Professor within KIP KSCX2-YW-G-030 project with the theme: „Simulation and applications of integrated cellular networks", at Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, **Tianjin** (China)(Prof. Jibin Sun) (**Fig.17**).
- **2014**: A severe stroke caused the cancellation of all foreign travels. However, Prof. Maria continued on-line some scientific collaborations with Technische Universität **Hamburg**

(TUHH), Institute of Bioprocess & Biosystems Engineering (Germany) (group of Prof. An-Ping Zeng). The collaboration resulted in several top articles in the field of ***in-silico*** design of **GMOs** (genetically modified micro-organisms) [Maria, 2021; Maria and Renea, 2021] (articles 26, 28, from the below list).

- **1990-2014. More than 30 invited conferences / seminars at prestigious universities. Among them are to be mentioned:**
- **Europe** ETH Zurich 1992-1997; RWTH Aachen 2004; U. Leeds 1996; U. Liverpool 1996; EPF Lausanne 1993-1996; U. Zagreb 2007; BASF Germany 1995; TU Erlangen 2000; TU Hamburg 2006,2009; TU Saarbrucken 1999; TU Braunschweig 2006; Univ. of Porto 1993,2000; Univ. Politecnica de Catalunya, Barcelona 1996; Univ. des Saarlandes 1999,2009; TU Stuttgart 1999; Ecole Nationale Polytechnique de Grenoble 1999; Ecole Nationale Polytechnique Montpellier 2000;
- **Canada** Queen's University Kingston 1994;
- **USA** Princeton University 1994; Texas A&M University 2002-2003;
- **China** Tianjin Institute of Industrial Biotechnology 2010;
- **România** Univ. Babes-Bolyai Cluj-Napoca (2013); Inst. of Biochemistry of the Romanian Academy (15 Jan. 2016).

TEACHING ACTIVITY (UNIVERSITY CAREER)

- **Full Habil. Professor (1999-2020)** at the Department of Chemical and Biochemical Engineering (**IChB**) (Lab. of Chemical, Biochemical and Biological Reactors) from the Polytechnic University of Bucharest (**U.P.Buc.**) (with completion of all teaching levels) (courses are mentioned in **Table 1**).
- **Supervisor of** PhD theses **(2008-present)** in **IChB** (Chemical, Biochemical and Biological Reactors) at **U.P.Buc.**

The rich technical-scientific activity of Prof. GM carried out in Romania, but also in the framework of several international projects at prestigious universities, was also reflected in his teaching activity within U.P.Buc. Thus are to be mentioned the following accomplishments:

- **Prof. GM is the successor, promoter, and developer of the Romanian school of reactors, and of chemical and biochemical reactions** engineering (kinetic modeling, ***in-silico*** design, optimization, and control of chemical, biochemical, and biological processes based on mathematical models, computing rules, and concepts specific to the (bio)chemical engineering { [7-8,10] ; book no. 12 from the belowlist}. While Prof. Raul Mihail (1920-1985) was the founder of the Romanian school of chemical and biochemical reactors, by publishing the first course of "Chemical Reactors" (1969-1971) in Romania (and 3rd in the world), and of "Bioreactors" (1987), Prof. GM was one of the valuable successors of his work, making a bridge over the years by developing a modern school of reactors and chemical and biochemical reaction engineering at U.P.Buc., by promoting it both at a theoretical and applied level, within the numerous research projects, publications [9], but especially within the applications in the chemical industry, materialized by addressing some innovative aspects (see section II.2.3 with some of his industrial achievements).
- **In short, as a member of the ICB Department of U.P.Buc.** [7,8,10] (**Fig. 2B**), **Prof. GM teach or supervised PhD, master's, and bachelor's courses/projects** in Chemical and Biochemical Engineering (1980-2020). Between 2006 and 2011, he was in charge with achievement and good results of the MSc. in Biochemical Engineering and Bioengineering at **U.P.Buc.** Between 1980 and 2021, he supervised more than **50** undergraduate (BSc.) projects, over **22** MSc. Diss., and of **11** PhD students (Romanian and foreign students) in Chemical and Biochemical Engineering at **U.P.Buc.**, ETH Zürich, and Texas A&M Univ. (USA). A list of doctoral and master's theses themes can be found in [7,9]. Some of his former PhD students are presented in (**Fig. 4**). Also, Prof. GM introduced several new courses (**Table 1**) in the Chemical and Biochemical Engineering study program (curriculum) at U.P.Buc. He has participated to a large number of national (27) and international (20) research projects on **IChB** as a director or key

researcher. Some are presented in chapter II.2.2 and in section "RESEARCH INTERNSHIPS, SCHOLARSHIPS, TEMPORARY POSITIONS ABROAD".

- **Creator of novel courses (and related manuals) introduced in the curricula of the (Bio)chemical Engineer at U.P.Buc.** Based on his strong research experience acquired when participating to research projects at esteemed universities in the EU and USA, and on his numerous publications, Prof. GM promoted in the field of chemical engineering education in Romania (at U.P.Buc.) various avant-garde courses and research directions, comparable with those developed in the EU, related to bioinformatics, chemical reactor operation safety, and others (see his courses in Table 1), with publishing the related teaching manuals/text-books (Table 2). Through all this, Prof. GM had and has a significant impact on the science and practice of the chemical and biochemical reactions engineering and reactors in Romania and world-wide.

Table 1. Teach **Courses** old, or newly introduced by Prof. GM in the Chemical and Biochemical Engineering curricula at U.P.Buc., by also ensuring the teaching support through the published text-books/manuals (see Table 2).
- Reactors and chemical and biochemical reactions engineering (BSC Degree in Chemical Engineering, from 1987); - Numerical and statistical methods for treatment of experimental (bio)chemical data, and to estimate the parameters of (bio)chemical process math models (BSC, MSC in Chemical Engineering) (new since 1997); - Quantitative analysis (based on mathematical models) of the operatingrisk of chemical processes and reactors. Numerical simulation of the consequences of a chemical accident (fire, explosion, toxic substances releases) (BSC, MSc in Chemical Engineering) (newly introduced in 2006); UPB.11.S.06.O.519; UPB.11.S.10.O.208; - Biochemical Engineering (BSC in Food Engineering, new since 2015); UPB.11.S.08.O.414; - Metabolic Engineering and Bioinformatics (MSC. in Food and Biochemical Eng.) (newly introduced since 2004); UPB.11.S.09.O.0406. (including *in-silico* design of GMO genetically modified microorganisms for industrial and medical use).

Table 2. **The textbooks** published by Prof. GM to support his newly introduced courses in Chemical and Biochemical Engineering curricula at U.P.Buc.
1. 1. Iordache and Maria, 1991. Book no. 1 from the below list of publications. 2. Maria, G., 2007. Book no.2 from the below list of publications. 3. Maria, G., 2008. Book no.3 from the below list of publications. 4. Maria and Luță, 2015. Book no.4 from the below list of publications. 5. Maria et al., 2016. Book no.5 from the below list of publications. 6. Maria, 2019. Book no. 10 from the below list of publications. 7. Maria, 2017, 2018. Book no. 7 and no. 8 from the below list of publications. **8.** Muntean, O., Bozga, G., Maria, G. et al., Chemical Reactors: Case studies, Lithography UPBuc., 1990, vol. 1 (334 pag), vol. 2 (293 pag.); CNCSIS= 180/78. (U.P.Buc.. library) **9. Maria, G.(coordinator),** et al., 2020. Book no.11 from the below list of publications. 10. **Maria, G., 2022,** Book no.12 from the below list of publications.

II. TECHNICAL-SCIENTIFIC ACHIEVEMENTS

II.1- FIELD OF RESEARCH:

chemical and biochemical engineering (ICB, IChB), bioinformatics.

Reactors , chemical, biochemical (enzymatic), and biological (cell cultures) reactions engineering; mathematical (kinetic) modeling, and numerical analysis (simulation) of these reactors with the aim of designing, optimizing and controlling their safe operation;

Mathematical modeling of the kinetics of chemical processes (catalytic and non-catalytic), of biochemical (mono- and multi-enzymatic), and of biological (cellular) processes. Statistical estimation of model kinetic parameters based on experimental data.

Risk analysis in the operation of chemical reactors and *in-silico* derivation (based on mathematical models) of the safe operation limits of the control variables; mathematical modeling and numerical simulation of the consequences-effects of a chemical accident scenario (fire, explosion, emissions of toxic substances into the environment, Domino effect).

Bioinformatics: math modeling of the dynamics (kinetics) of various cellular metabolic processes, namely: i) individual gene expression regulation (GERM), ii) regulation of protein synthesis, iii) simulation of cellular genetic regulatory circuits (GRC), iv) simulation of the central carbon

metabolism (**CCM**) in living cells, in order to ***in-silico*** (based on structured, modular, deterministic mathematical models, with continuous variables) design of genetically modified micro-organisms (**GMOs**) with desired characteristics, with industrial and medical applications (metabolic engineering; computational biology). Based on all his published works in these topics, prof. GM has made fundamental theoretical contributions in several frontier fields, namely "systems biology" and "synthetic biology", "bioinformatics", "computational biology".

Math modeling of the drug release kinetics in biological fluids for ***in-silico*** design of optimized controlled (programmable) release systems.

Chemical energetics. I) Chemical storage of energy (H2) and its transport at long distances; ii) production by non-conventional catalytic processes (via methanol) of hydrocarbons (olefins, aromatics), and of synthetic gasoline from cheap sources, such as inferior coal and renewable biomass].

Chemical engineering, chemical reaction engineering	Protein synthesis regulation (gene expression kinetics); simulation of the genetic regulatory circuits in living cells,
Metabolic engineering, computational biology	Systems biology, bioinformatics
Biochemical engineering, biochemical reaction engineering	Modelling the dynamics of genetic regulatory circuits
Chemical, biochemical and biological reactors (modelling, optimization, control)	Wastewater biological treatment (kinetic modeling)
Kinetic (mathematical) modelling of chemical, (bio)chemical, and biological processes	Risk analysis and ecological impact of risky chemical reactors (determination of critical operating conditions, simulation of the reactor run-away conditions). Optimized operating policies of risky chemical reactors.
Process identification, statistical estimation, data numerical treatment	Simulation of chemical accidents consequences and effects
(Bio) chemical process analysis and optimization	Chemical energetics (chemical storage of the hydrogen energy)
Enzymatic processes and catalytic process kinetic modelling	Controlled drug delivery (kinetics modelling; system delivery design).
Modeling the dynamics and regulation of metabolic processes in living cells (cell simulators)	

II.2- THE RESULTS OF HIS RESEARCH ACTIVITY:

The results of his research activity in its fields (II.1) can be found in:

- **II.2.1. P**ublication productivity
- **II.2.2. R**esults obtained in the framework of international research projects
- **II.2.3. M**ajor industrial realizations
- **II.2.4.** Published **T**heoretical contributions (basic / fundamental research)

II.2.1.- Summary of his publishing activity

The numerous theoretical (fundamental) but also practical (industrial) achievements of prof. G. Maria are also reflected through a rich publishing activity. His main publications include: 20 books (with ISBN) and university textbooks of **IChB** and bioinformatics (see his list of publications [7-9] and the below selection). In short, scientific productivity materialized in:

-.- **8** ISBN books in Romanian,
-.- **7** ISBN books in English in the USA,
-.- **5** university textbooks (U.P.Buc.),
-.- **12** book chapters with ISBN abroad [7-9],
-.- main author of **157** papers in ISI esteemed journals (over **50** in top **IChB** publications)
-. (co-)author of **82** papers in international scientific conferences [9]

All the above books, with the exception of the university textbooks (written in collaboration) have Prof. GM as sole author, or as main author (coordinator). His publications are well cited (**Hirsch index 23**, **I10 index 57**, with over **1800 citations**). He also published a significant number of papers (**over 15**) in the annals / scientific bulletins of the universities. He registered high / top scores in the Romanian classification system (MEdC-OMs-2011).

II.2.2. Results in the framework of international research projects

He participated to more than **20** international research projects as director and/or key investigator. Among them are to be mentioned:

- **1992-1997. Swiss Dept. of Energy project NEFF 505 ("Saisonale Speicherung von Elektrizitat mit Chemisch Gebundenem Wassertsoff", "Seasonal storage of electricity using chemically bonded H2") at ETH Zürich and Paul Scherrer Institut Villigen (Switzerland).**

Impact. The project was developed at a theoretical and experimental level, being tested in a medium-sized pilot plant (2 fixed-bed catalytic reactors connected in series) at the Paul Scherrer Institute Villigen (Switzerland) in cooperation with the DFG (Germany) and Vinci (France) . Prof. GM was responsible for i) the numerical treatment of the experimental data automatically on-line recorded during long times-on-stream operation (weeks) of the pilot, in order to develop the kinetic models of the involved catalytic processes and, ii) the ***in-silico*** technological design (based on math models) of the pilot plant. The project aims to transport chemically stored hydrogen between continents. Thus, H2 is stored by hydrogenating toluene (TOL) to methylcyclohexane (MCH), then MCH is transported to the recipient where it is dehydrogenated to TOL (thus recovering H2). TOL is returned to the H2 source and the cycle is resumed. Dr. Maria handled the kinetic modeling and design of the series of fixed bed catalytic reactors used for TOL hydrogenation, or for MCH dehydrogenation. [Maria et al., Chem. Eng. Sc. 51, 2891-2896 (1996). doi:10.1016/0009-2509(96)00170-4].

- **1999 – 2001 Director of NATO Scientific Division Grant no. 974850-99/1999-2001. with the theme „Theoretical and lab-/pilot-scale studies on model-based optimization of biological treatment of municipal wastewaters". Partners: Polytechnic University of Bucharest (UPBuc.), Inst. of Environmental Engineering ICIM Bucharest, University of Porto (Portugal).**

Impact. Prof. GM contributed with the mathematical modeling and dynamic simulation of the series of 3 bioreactors included in the experimental pilot plant at of ICIM, and with optimization of their safe operation. The positive results were validated, generalized and published [Maria et al., Comp. Chem. Eng. 24, 1713-1718 (2000). **[Two]**:10.1016/S0098-1354(00)00447-6].

- **2002 – 2003. Guest professor at Texas A&M University (TAMU, College Station, Texas, USA), Department of Chemistry and Cellular Biology, stipendium from the National Institute of Health (NIH, USA) for the project NIH PAL-GM63958/2002-2003: „Kinetic simulations of minimal living systems", and for the NIH project EES-GM64650/2002-2003: „Molecular recognition in dendrimers based on melamine - Kinetics of programmable drug release in human plasma", (Prof. E. Simanek).**

Impact. In project PAL-GM63958 / 2002-2003, theoretical studies of prof. GM focused on development of reduced mathematical (kinetic) models for simulating the regulation of protein synthesis in living cells. This involved math modeling of the kinetics of individual gene expression regulatory modules (**GERMs**), and of the genetic cellular regulatory circuits (**GRCs**) **(e.g. operons expression**, genetic switches acting as a molecular biosensor, etc.), and of the enzyme syntheses in bacteria of industrial interest. The research was developed at TAMU by Prof. GM within the framework of a grant offered through competition by the National Institute of Health (NIH-USA, 2002-2003). Prof. Maria proposed new approaches to mathematical modeling of cellular systems by an analogy with the numerical algorithms and concepts used in the (bio)chemical engineering (**IChB**), and in the nonlinear systems theory. The positive results of this project were subsequently published (eg modeling the dynamics of the metabolism regulation of heme synthesis in mitochondria; Hudder, Maria, 2002 [14]). Such dynamic simulators of cellular **GRCs** are useful to evaluate the cell metabolic fluxes further used for the *in-silico* design of **GMOs** with applications in the biosynthesis industry, medicine, environmental engineering, etc. [monographs no. 7-8 from the below list].

Impact. Within the EES-GM64650 / 2002-2003 project, theoretical studies of prof. GM focused on the development of extended and reduced kinetic models to numerically simulate the dynamics of drug release over time in biological fluids, by using a chemical release control based on the use of bio-supports of melamine-based multivalent dendrimers. The research was developed by Dr. GM in the framework of a NIH-USA grant (2002-2003), by using the experiments carried-out at TAMU. The results were published in top journals [Zhang, Maria, et al., Jl. American Chem. Soc.. 125, 5086-5094 (2003)]. The research was later continued in Romania within an EU project (namely the below ZEOMED) (**Fig.11**)

- **2011-2014 EU-POSCCE project "New mesoporous alumino-silicate matterials for the controlled release of drugs in biological fluids", ZEOMED).**

Impact. The experimental and theoretical studies carried out as part of international collaborations by Prof. GM (that is development of mathematical models of the chemical-diffusion kinetic process during the drugs release from porous solid supports) led to obtaining math models and software necessary for the *in-silico* design of controlled release drugs, of an adjustable release time. Numerous functionalized supports (porous silicates MCM-41, **Fig.12**) were tested, by using many test drugs (cytostatics, anti-TBC, sulfonamides, antibodies, etc.). The results were published in top journals [9] and in his book no. 4 from the below list.

- **2006 (July-Aug.) project DFG-578 /2006 at TU Braunschweig (Germany), Dept. of Bioengineeeirng (Prof. W. Deckwer), with the theme: „The Development of Biotechnological Processes by Integrating Genetic and Engineering Methods".**

Impact. The Prof. GM's studies within this project focused on the development of structured, reduced, modular mathematical (kinetic) models for simulating the dynamics of essential biochemical processes in living cells, namely the central carbon metabolism (**CCM**). The practical applications led to the development of a structured modular model to numerically simulate the dynamics of **[mercury-operon expression]** regulation in *E. coli*, further used for the *in-silico* design of **GMOs** with a higher efficiency in the removal of mercury from wastewater, followed by its recovery (Maria and Luta, Comp. Chem. Eng., 58, 98-115 (2013). DOI: 10.1016/j.compchemeng.2013.06.004) and the book no. 8 from the below list.

II.2.3. Major industrial achievements

Prof. GM was involved in many major research projects with practical achievements at the industrial level, both in Romania and abroad (Switzerland). These important realizations are summarized below.

a). - MTO/MTG industrial plant. Between 1981-1991, dr. GM worked as a key engineer-researcher at ICECHIM - Chemical and Biochemical Energetics Institute Bucharest (**IECB**), (Bio)catalysis group. Here, Dr. GM was in-charge with: i) mathematical modeling of the kinetics of a very large number of catalytic processes tested at a laboratory / industrial pilot scale, and ii) with the technological design, construction and put into service of an industrial pilot plant at the Brazi Petrochemical Works (Ploiesti, Romania)[5,6] for testing novel, non-conventional technologies for the production of hydrocarbons (olefins, aromatics), and of synthetic gasoline from cheap sources (via methanol), such as inferior coals or renewable biomass (books no. 9 and 11 from the below list).

Impact. In this context, must be underlined the remarkable, exceptionally valuable, and pioneering studies conducted by Prof. GM regarding the mathematical modeling of the kinetics of novel catalytic processes which, finally they led to the development of novel, non-conventional, revolutionary (avant-garde) technologies in the field of valorization through methanol of multiple renewable and cheap resources respectively, the conversion of methanol to olefins **(MTO)**, to synthetic gasoline **(MTG)**, to aromatic hydrocarbons **(BTX),** or to propylene **(MTP),** by using zeolitic/silica catalysts modified and tested by ICECHIM-IECB. These kinetic studies were published by Dr. Maria in top **IChB** journals, and they represented the foundation for the design and construction of a demonstrative industrial plant for the above mentioned processes at the Brazi Petrochemical Works (Ploiesti, Romania), activities in which Prof. GM had a major / key contribution [5-8]. The MTO/MTG industrial plant (**Fig. 5a-b**), with the characteristics presented in [5-7] (and in books no. 9 and 11 from the below list), **includes two chemical catalyst fluidized bed reactors](FBR).** The micro-spherical catalyst presents a continuous circulation by means of a pneumatic transport between the main **FBR** (where the MTO, MTG, or other desired reactions are conducted), and the secondary **FBR** used for the continuous regeneration of the partially coked catalyst (see details in [5,6]) . At that time (1980-1985), the industrial plant mentioned above was the first in the world to test MTO/MTG processes by using this novel technology. It was only a similar plant of Mobil Oil (USA) who was operated in New Zealand, but of a much simpler construction (a plant with 5 parallel multi-tubular fixed-bed catalyst reactors, with discontinuous catalyst regeneration)[6]). Later, industrial MTO/MTP plants were built by UOP/Hydro co. in Germany and in China, but using different technologies [5,6] (see also the books no. 9 and 11 from the below list).

By using this industrial plant, and the experimental data provided by IECB, Prof. GM developed kinetic models and tested numerous catalytic processes during 1985-1992, respectively for: i) the selective alkylation of C4 olefins with methanol; ii) alkylation of benzene or ethyl-benzene with ethylene to obtain higher aromatic hydrocarbons; iii) ethanol conversion to olefins; iv) methanol conversion to BTX (benzene, toluene, xylenes)[5-6] (see also books no. 9 and 11 from the below list).

For such an exceptional achievement, Prof. GM received (as a research/key design engineer, as part of the research/design team involved in this project of great scope) the "Nicolae Teclu" Award of the Romanian Academy in 1985 (**Fig. 6**).

b).- Pilot plant for the chemical storage of energy (via hydrogen) and its transport at long-distances. In 1992, Dr. Maria chose to accept an invitation and he came to Switzerland to work as an Assistant Professor (Oberassistent Klass 18) with the Polytechnic University ETH Zürich (Switzerland), in the "Process Systems Engineering" group of the late Prof. David WT Rippin (Chemical Engineering Dept.). Here, Prof. GM was involved in teaching activities (supervising,

or co-supervising several PhD, or Master's Degree students). But, Dr. Maria also actively participated as a key [investigator/researcher] to the materialization of several important research projects of the group, all in the field of (bio)chemical engineering (**Fig. 7**).

Impact. One of these industrial-scale projects (NEFF) concerns the technological design and commissioning by prof. GM of a medium-sized, fully automated pilot plant consisting of a system of two fixed-bed catalytic reactors linked in series (**Fig. 8**), at the Paul Scherrer Institute (Villigen, Switzerland, 1992-1996), in cooperation with DFG Germany, and Vinci co. (France) aiming to study and test of a novel, avant-garde, process. The application concerns the chemical storage of hydrogen and its transport between continents. Thus, H2 is stored by catalytic hydrogenation of toluene (TOL) to methyl cyclohexane (MCH). MCH is then transported (by sea) to the recipient where H2 is released by means of the catalytic dehydrogenation of MCH to TOL. The toluene is then returned to the H2 source, and the cycle is resumed. Prof. GM was in-charge with the kinetic modeling of the two catalytic processes, aiming to realize the technological design and the on-line control of the pilot plant alternatively used for TOL hydrogenation, and for MCH dehydrogenation, respectively (Maria et al., *Chem. Eng. Sci. 51,* 2891-2896 (1996). **[doi]:**10.1016/0009-2509(96)00170-4).

c- In-silico optimization of the safe operation of some high-risk chemical catalytic reactors. Another research project where Prof. GM came up with the valuable and innovative solutions was those developed at ETH Zürich (Switzerland). The project aimed to ***in-silico*** determine (based on mathematical models) the optimal safe operation policies of some high-risk catalytic reactors in the pharmaceutical industry, operated by CIBA /Novartis (Basel, Switzerland, 1992-1997). **Impact.** The process in question refers to the aceto-acetylation of pyrrole with diketene in homogeneous catalysis (with pyridine), a particularly dangerous reaction which, out of control, produced frequent explosions of the industrial reactor at CIBA (NOVARTIS) - Basel (Switzerland) . Prof. GM managed to solve this problem by including in the numerical procedure used to determine the optimal operation policy of this catalytic reactor of an original probabilistic index (parameter), that expresses, in numerical terms, the process runaway risk and the reactor explosion risk, due to the presence of random fluctuations of the control parameters. See his top publications: i) Maria et al., Chem. & Biochem. Eng. Q. 24(3), 265-281 (2010); ii) Maria and Dan, Comput. & Chem. Eng. 35*,* 177-189 (2011). **[Doi]:** 10.1016/j.compchemeng.2010.05.003; iii) Maria and Dan, Asia-Pacific Jl. Chem. Eng., 7*,* 733-746 (2012). DOI: 10.1002/apj.625; iv) Dan and Maria, Chem. Eng. & Technol., 35(6), 1098-1103 (2012). DOI: 10.1002/ceat.201100706 [7-9].

d- Optimizing an existing industrial plant. Right from the first years of his career, Dr. GM was involved in research topics aiming at optimize the existing industrial reactors in Romania. One of these applications refers to the optimization of the hydrocarbons pyrolysis reactor at Arpechim Pitești Petrochemical Works, Romania (1980-1991).**Impact.** The study focused on the numerical simulation, by using complex mathematical models, of the radiative heat transfer in the pyrolysis furnaces coupled with the numerical simulation of the dynamics and performances of the tubular hydrocarbons pyrolysis reactor (120 m length, 0.3-0.5 m diameter), immersed in the pyrolysis furnace (9×3×6 m) aiming to improve the reactor performance. To this end, the study aimed to optimize the elliptical shape of the tubular pyrolysis reactor in order to intensify the heat transfer **(Fig. 9a-b)**. See his works: i) Mihail and Maria, Revista de Chimie(Bucharest) 32, 988-994 (1981); ii) Ibidem, Revista de Chimie 33, 157-161 (1982); iii) Ibidem, Int. Journal of Heat & Mass Transfer 26*,* 1783-1789 (1983); iv) lot of subsequent papers **[9].**

II.2.4. Theoretical contributions (fundamental research) with major impact on his research field

1.¤ Reactors and the chemical and biochemical reactions engineering.

i.- Kinetic (mathematical) modeling of the dynamics of catalytic processes [chemical, biochemical (multi-enzymatic), or biological (cellular metabolic processes, that is metabolic syntheses, individual gene expression **GERM**, cell genetic regulatory networks **GRC**)] for engineering purposes. **Impact.** Proposal of a very large number (over 40 [7]) of complex kinetic models for various catalytic, processes (chemical, enzymatic, and cellular biological) (books no. 6-8,11 in the below selection list; [7-9,13,14]). Proposal of novel original numerical algorithms (MMA, MMAMI, **Table 3**) to estimate the parameters of the (bio-)chemical processes kinetic models, by solving the associated nonlinear programming problems **NLP** (with continuous variables), and nonlinear programming problems with mixed continuous and integer mixed variables **MINLP** [7-8,12]. Proposal of several original statistical tests for reducing complex kinetic models, in order to facilitate the further chemical engineering calculations, by grouping the redundant parts of the model (**Table 3** ; book no. 10 from below list).

ii.- Mathematical modeling and numerical simulation of chemical, biochemical and biological reactor dynamics **Impact.** These tools are used for the design, optimization, and control their safe operation.

Development of numerical algorithms for the multi-objective optimization (Pareto or non-Pareto) of various reactor types of chemical, biochemical (multi-enzymatic), or biological (cell cultures) [7-9]. Development of an expert system able, for a given enzymatic process with known kinetic model, to select from a database the most suitable reactor type, and to optimize its operating regime (**Fig. 10**, right).

2.¤ Quantitative analysis (based on mathematical models) of the thermal runaway risk of a chemical reactor (especially the complex catalytic ones where exothermic reactions are conducted).

a. –Proposal of **novel probabilistic indicators** for evaluating the runaway risk of exothermic chemical processes conducted in various chemical reactor types. Proposal of novel numerical procedures to ***in-silico*** estimate the safe operation boundaries of various chemical reactors, in order to optimize their safety operation [7,9] (see point "c" in chapter "Major industrial achievements");

b.- Technological risk *in-silico* assessment of chemical processes and of their environmental impact, by using mathematical models. Numerical simulation and evaluation of chemical accident scenarios generated by the poor control of chemical reactors. The assessment, by using the numerical simulation, of the consequences (human/constructions fatalities) in the accident spot, or of the Domino effects, etc. Prof. GM wrote and published the first monography / teaching book in Romania (2007) in this field (book no. 2 from the below selection list);

c.- Proposal of a **combined procedure**, experimental (DSC calorimetry), as well as a numerical (MIP), to be used for the quick estimation of the global kinetics and risk of a new chemical process [Maria and Heinzle, Jl. Loss Prev. Proc. Ind. 11(3), 187-206 (1998); Comput. & Chem. Eng. 23, S71-S74 (1999)];

d.- Proposal of **novel numerical algorithms** to estimate the **critical operating conditions** (safe operating boundaries) for various types of chemical reactors, where hazardous exothermic chemical reactions are conducted. These algorithms use dynamic mathematical models of the analysed process/reactor, and determine the conditions leading to the divergence of the operating parameters from their nominal values, in the presence of random fluctuations of the control variables [7-8].

3¤ Modeling the kinetics of drug release in biological fluids. Proposal of mathematical models to numerically simulate the dynamics of drug release from porous (functionalized) solid supports in biological fluids, to be further used to ***in-silico*** design of drugs with an optimized controlled release (**Fig. 11-12**, book no. 4 from the below selection list).

4¤ Bioinformatics. In 2002, Prof. GM won a research grant from the US National Institute of Health (NIH) and he came to Texas A&M Univ. (TAMU, College Station), Dept. of Chemistry, Biochemistry and Cell Biology, to work as a key researcher in two NIH-funded projects (**Fig.13**), respectively: PAL-GM63958/2002-2003: "Kinetic simulations of minimalist cellular systems" and EES-GM64650 / 2002-2003: "Molecular recognition in melamine-based dendrimers - Kinetics of programmable drug release into human plasma from dendrimer supports". In a short time, prof. GM brought significant and essential contributions in both subjects, namely: i) cellular enzyme reaction engineering and bioinformatics, by developing kinetic models for some essential metabolic processes in living cells, and ii) developing kinetic models for a controlled drug release in human plasma. The published contributions in this topic (books no. 6-8 in the below list; papers reviewed in [7-9,13,14]) refer to:

i.- Proposing a **novel, modular math modeling framework** and a holistic approach (**WCVV** "variable volume whole cell") for the development of dynamic mathematical models of essential cellular metabolic processes, especially those related to simulation of the central carbon metabolism **(CCM)** **(Fig. 14)**, of individual gene expression **(GERM),** and of genetic regulatory circuits **(GRC)** responsible for regulating the essential cellular metabolic syntheses. These dynamic cell models are then used for the ***in-silico*** design of **GMOs** used in industrial biosynthesis, medicine, etc. (books no. 6-8 from the below list, and [7-9,13,14]).

ii.- Development, in the framework of international collaborations, of numerous applications of these cell simulators aiming the *in-silico* design of **GMOs**, (books no. 6-8; [7-9,13,14]). For example: a) *in-silico* design of **GMO** *E.coli* in order to maximize the mercury removal from wastewaters **(Fig. 15,** left); b) *in-silico* design of **GMO**-modified *E.coli* in order to maximize the tryptophan production **(Fig. 15,** right); iii) *in-silico* design of **GMO** modified *E.coli* to maximize the succinate production **(Fig. 14, bottom),** and others.

5¤ Contributions to basic numerical calculations and statistical algorithms.

Prof. GM has developed new numerical methods for solving non-linear optimization/estimation problems used to solve difficult problems related to identifying (bio)chemical kinetic models, and to optimizing (bio)chemical reactors. The most important ones are mentioned in **Table 3**.

Table 3. The main numerical algorithms developed and published by prof.GM [7-8].

MMA, MMAMI [12] – An adaptive, random iterative numerical procedure to search for the global extremum of a nonlinear, multi-modal objective function (convex or non-convex, in the presence of multiple constraints of all types), applied to the identification of complex (bio)chemical kinetic models. Later, Dr. Maria extended the applicability of the MMA procedure to solve NLP problems, by proposing the MMAMI numerical algorithm able to successfully solve MINLP optimization problems. Dr. Maria chose to donate the right to use these routines to several universities: TU Saarlandes (1999), TU Karlsruhe/DECHEMA (Germany) (2000) and Tianjin Inst. Ind. Biotehnology (China) (2010).

CPEMR – a combination of numerical algorithms for simultaneous estimation and reduction of a complex (bio)chemical kinetic model. The procedure is based on classical statistical tests, but also on an original one [7-8](Maria, G., Canadian J. Chem. Eng. 67, 825-832 (1989)).

KINEXP – an expert system for identifying a (bio)chemical kinetic model using experimental kinetic data, but also an original procedure for transferring information from kinetic data banks ("artificial intelligence" type) [7-8] (caption **Fig. 10**, Left). KINEXP also uses the method of gradually reducing the structure of the kinetic model by using "lumping" techniques (by grouping species/reactions), with preserving the reaction invariants (caption **Fig. 11** and book no. 10 from the below list).

MIP – a numerical algorithm for the rapid (direct) estimation of the kinetic model of a (bio)chemical process by using isothermal kinetic experimental data, but also an algorithm to transfer information from a kinetic data bank [7-8] (Maria & Rippin, *Comput. & Chem. Eng. 21*, 1169-1190, 1997).

RSA – an original statistical test for determining the redundant part of a kinetic (bio)chemical model (book no. **10**).

GHSM- A Numerical Procedure for Solving Nonlinear Mathematical Models by Using a Generalized Search Interval Halving Method (Maria and Smigelschi, 1986)[7,9].

DSC-MIP. A combined experimental method (DSC calorimetry), with a numerical algorithm (MIP) for identifying the global chemical kinetic math models (see chapter. II.2.4, issue 2-c).

Proposal of a numerical procedure for detecting the invariants of complex chemical reactions. The aim of this numerical procedure is to reduce extended kinetic models by using lumping techniques (book no. 10 from the below list), to make them easier to be used in engineering calculations. A successful exemplification was made in the case of a complex kinetic model (64 reversible reactions, and 16 species) used to simulate the dynamics of chemically controlled release of drugs from a **[multivalent dendrimeric support]**. The kinetic model was finally reduced to only 4 reversible reactions that include 5 groups of conformational isomers, with rate constants estimable from the experimental data [7-8] (see the reference from **Fig. 11**). The proposed technique also allows the evaluation of the intrinsic kinetic constants (from the extended models, difficult to be estimated), based on the apparent ones (used in reduced models, easily to be identified).

IMPACT ON HIS FIELD OF RESEARCH

Prof. GM is an esteemed scientist in Romania, with impressive theoretical and practical achievements, all these having a major impact on the science and practice of Reactors and Chemical and Biochemical Reaction Engineering in Romania and world-wide. Thus:

i. He led courses and coordinated studies for PhD Theses, Master's Degrees, Bachelor's Degrees in Reactors, and Chemical and Biochemical reaction engineering (1980-2021) (see chapter "**TEACHING ACTIVITY**").

ii. He introduced new courses (**Table 1**) in the Chemical Engineering curriculum at Polytechnic University of Bucharest (U.P.Buc.), to bring it up to date with that of the EU, and he wrote and published the related teaching text-books (**Table 2**);

iii. He introduced the first course and published the first teaching book in Romania on the topic of quantitative assessment (based on mathematical models) of operation risk of chemical plants/reactors, and on ***in-silico*** prediction of the extent of consequences and effects of a chemical accident hypothetical scenario (book no. 2 from **Table 2** and from the below selection list).

iv. He had and still has an impressive publishing activity in **IChB** (see chapter II.2.1).

v. He had many remarkable achievements at a theoretical or industrial level, in Romania, but also abroad (see chapters II.2.2 and II.2.3).

vi. He has published numerous theoretical contributions (fundamental research) with a major impact on his research field (chapter II.2.4).

INTERNATIONAL RECOGNITION

• **Co-chair or member of the scientific committees of 16 international conferences.** Among them are to be mentioned: *5th Int. Conf. on Computational Bioeng.* (ICCB-5), 11-13 September, 2013, Leuven (Belgium); *ROMPHYSCHEM 15-th Intl. Conf. of Physical Chemistry*, 11-13 Sept., 2013, Bucharest; 13-th Conf. *Academic Days* Timişoara, June 13-14, 2013; ESCAPE-17 (*European Symp. Computer Aided Proc. Eng.*), 27-30 May 2007, Bucharest, etc.

• **IMore than 30 nvited lectures / seminars in the field of IChB at esteemed universities,** namely: ETH Zurich (1992-1997), RWTH Aachen (2004), U. Leeds (1996), U. Liverpool (1996), **EPF Lausanne (1993-1996)**, U. Zagreb (2007), **BASF Germany (1995)**, TU Erlangen (2000), TU Hamburg (2006,2009), TU Saarbrucken (1999), TU Braunschweig (2006); Univ. of Porto (1993,2000); Univ. Politecnica de Catalunya, Barcelona (1996), Univ. des Saarlandes (1999,2009), Ecole Nationale Polytechnique Grenoble (1999), Ecole Nationale Polytech. Montpellier (2000); **Queen's Univ. Kingston**, Canada (1994), **Princeton Univ. (1994), Texas A&M Univ. (2002-2003)**, Tianjin Inst. Ind. Biotechnology, China (2010), Univ. Babes-Bolyai Cluj (2013); Inst. Of Biochemistry of the Romanian Academy (15 Jan. 2016), etc.

• **More than 10 invited plenary lectures at various international conferences.** Among them are to be mentioned: 5-th European Symp. Computer Aided Proc. Eng., June 11-14, 1995, Bled (Slovenia); 20-th Croatian Meeting of Chemists & Chemical Engineers, Feb. 2007, Zagreb; 12-th Conf. Academic Days, Timişoara (RO), 26 May 2011; 15-th ROMPHYSCHEM, Intl. Conf. Physical Chemistry, 11-13 September, 2013, Bucharest; 12-th ELSEDIMA International Conference on Safety Engineering, 18 Sept. 2014, 26 May 2016, 17 May 2018, Cluj-Napoca (RO), etc.

• **Visiting professor in the framework of bi-lateral collaborations/temporary positions/seminars at numerous prestigious universities,** namely: ETH Zurich 1992-1997; Queen's Univ. Kingston (Can.) 1994; U. Leeds 1996; U. Liverpool 1996; TU Saarbrucken (1999); TU Erlangen (2000); RWTH Aachen 2006; TU Braunschweig (2006); TU Hamburg (2009); U. Zagreb 2007; Princeton Univ. 1994; Texas A&M Univ. 2002-2003; Tianjin Inst. Ind. Biotechnol. 2010, etc.

• **Voluntary activities within EFCE** (European Federation of Chemical Engineering) and CAPE (Computer Applications in Chemical Engineering): i) The representative of Romania in the framework of the 1st EU Congress of Applied Biotechnol., 25 Sept. 2011 (Berlin), and in 1995 to the EFCE conference in Davos. ii) The initiator and member of the scientific committee for the Symposium "Modelling for improved bioreactor performance-3", 21-23 Sept. 1995, Poiana Braşov, RO); iii) Co-chairman Intl. conf. ESCAPE-17/CAPE, Bucharest, 27 May 2007 (**Fig. 18**); iv) Key readings at EU ESCAPE conferences: 1992 Toulouse; 1995 Bled; 1996 Rodos; 1999 Budapest.

• **Editorial activities (voluntary).** Member of the scientific committee or editorial board of the following scientific journals (ISI/Scopus): 1) Chemical & Biochemical Engineering Quarterly (Croația); 2) Revista de Chimie (Bucharest); 3) Revue Roumaine de Chimie (Bucharest); 4) The Scientific Bulletin of Polytechnic University of Bucharest (Series Chemistry & Materials Science); 5) Bulletin of Romanian Chemical Engineering Society; 6) ECOTERRA Journal of Environmental Research and Protection (Romanian Soc. of Environmental Sciences and Engineering, Cluj, ROU).

• **International scientific reviewer (volunteer)** for a very large number (over 25) of scientific journals in his research field. Among them, there are to be mentioned:
AICHE Journal, Analytica Chimica Acta, Bioprocess and Biosystems Engineering, Canadian Journal of Chemical Engineering, Chemical Engineering Science, Chemical Engineering Journal, Chemical & Biochemical Engineering Quarterly, Chemical Engineering Communications, Computers & Chemical Engineering, Environmental Science and Technology, Food Technology and Biotechnology, Ind. Engineering Chemistry Research, Journal of Process Control, Jl. Biotechnology, Jl. of Bioscience & Bioeng., Journal of Molecular Catalysis B: Enzymatic, Journal of Petroleum and Gas Engineering, Revista de Chimie (Bucharest), Revue Roumaine de Chimie (Romanian Academy); Microporous and Mesoporous Jl.; Biocemical Eng. Jl.; Chemical Eng. Jl.; Sc. Bull. Univ. Politehnica Bucharest ,etc.

• **(Volunteer) activity as an expert (evaluator) in the fields of: IChB, bioinformatics, industrial chemical risk, analysis** for various (inter)national scientific programs: EU (FP-6, Brussels), SNSF (Switzerland, 2009), Croatia (2006), Biotech (RO, 2006).

AWARDS AND HONOURS

- 1974, Gold medal at the 6th International Chemistry Olympiad , of highschool students, IChO (11 countries)[1-3,7] (**Fig. 1A**);
- 1985, "Nicolae Teclu" Award of the Romanian Academy for kinetic studies, scale-up, design and commissioning of an industrial plant for testing novel, non-conventional processes (MTO, MTG, etc.) at the Brazi Petrochemical Works (Ploiesti, Romania) [5,6,7-9] (**Fig. 5a-b, Fig. 6**);
- 2006, Diploma of Excellence in Research, granted by the Romanian Federation of Biomedical Engineering (**Fig. 1B**);

- 2010-2021, **20** awards from the Romanian Research Agency UEFISCDI, for top papers published in top journals (Q1-Q2);
- 2019, unanimously elected as Corresponding Member of the Romanian Academy (Chemical Sciences section) (**Fig. 3**);
- 2020, designated as President of the Chemical and Biochemical Engineering Commission (**IChB**), within the Chemical Sciences section of the Romanian Academy (**Fig. 16**). See also books no. 11 and 12 from the below list, authored by Pof. GM.
- tribute papers and booklets dedicated to Prof. GM [3,7,8a-b,10].
- Nominated (position 1 out of 3 proposals) for the Grand Prize of the Grand National Masonic Lodge in Romania (21st June 2023 [15-16].

ACTIVITY WITHIN THE ROMANIAN ACADEMY

• **Head of a Specialized commission.** From January 2020, Prof. GM is the president of the Chemical and Biochemical Engineering Commission (**IChB**) within the Chemical Sciences section of the Romanian Academy. This consists of a group of researchers and university professors with outstanding results in the **IChB** research field, a group created with the purpose of analysing and reflecting on the dynamics of the **IChB** field, and to generate analyses on the evolution of **IChB** at an EU, world-wide, as well at a national level. All these have as a result formulation of books, or papers including studies, analyses, ideas, and strategies for the sustainable development of **IChB** in Romania. Two of such works dealing with the future **IChB** in the EU and and in Romania were published in 2020 (**Fig. 16**) by the **IChB**-AR Commission, respectively monographs no. 11 and no. 12 from the below list.

 Editorial activities. (see also the above paragraph **„Voluntary editorial activities"). ** Prof. GM is a member of the scientific/editorial board of 5 ISI journals in his field of research. Among them are: ***Revue Roumaine de Chimie (Bucharest)***, edited by the Romanian Academy, and **Chemical and Biochemical Engineering Quarterly** (edited by the Chemistry and Chemical Engineering Society of Croatia).

OTHER ACTIVITIES (RESPONSIBILITIES)

• Member of the National Council for the Attestation of University Titles, Certificates and Diplomas (CNATCDU), Chemistry and Chemical Engineering section (2011-2012);

• Member of the Romanian Society of Chemical Engineering, of the Romanian Society of Chemistry, of the Romanian Society of Bioengineering and Biotechnology, of the Alumni association of former DAAD scholars (Germany), of the National Society of Environmental Science and Engineering (Romania), of EFCE (national representative in 1995 and 2011);

• Member of the Council of Faculty of Applied Chemistry of Polytechnic University of Bucharest **U.P.Buc**. (2012-2014);

- Assistant Professor at ETH Zurich (Dept. of Chemical Engineering, 1992-1997);

- Research stipendium of the National Institute of Health (NIH) USA at Texas A&M University, Dept. of Chemistry, Biochemistry, and Cell Biology (College Station, TX, USA)(2002-2003).

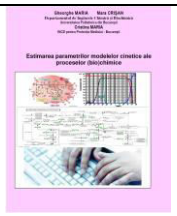
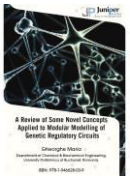
PUBLISHED WORK (SELECTION)

The almost complete list of publications by Prof. Dr. Eng. GM can be found at his personal web page from Research-Gate = **https://www.researchgate.net/profile/Gheorghe-Maria-2**
Or at his web-page from Googleschoolar.

ISBN BOOKS

(selection of 20 books published in Romania and USA; 5 university textbooks; 10 chapters of ISBN books in English)

Libraries where the books are available: AR = Romanian Academy; UPBuc. = Polytechnic University of Bucharest.

	**1. Iordache, O., Maria, G., Corbu, S., Statistical modeling and the estimation of parameters for chemical processes, Romanian Academy (RA) publ., Bucharest, 1991, 240 pages (ISBN 973-27-0195-1) (AR; UPBuc. library);** **Impact:** the first monograph in Romania that presents a systematic review on numerical optimization algorithms, and statistical tests used to identify and evaluate the quality of mathematical models of (bio)chemical processes (AR, UPBuc.). (in Romanian).
	**2. Maria, G., The quantitative risk assessment of chemical processes and math modeling of accident consequences, Printech, Bucharest, 2007 (630 pages), ISBN 978-973-718-667-6(UPBuc. library);** **Impact:** the first monograph in Romania that presents (with solved case studies) numerical algorithms and mathematical models used to assess the runaway risk when operating chemical reactors, as well as to assess the consequences and effects of a chemical accident scenario (fire, explosion, toxic compounds releases in the environment). Course support (teaching textbook at U.P.Buc. (Bachelor BSC, MSC.) (U.P.Buc. library). . (in Romanian).
	**3. Maria, G., The statistical treatment and correlation of experimental (bio)chemical data. DStatistical dstributions and estimators, Printech, Bucharest, 2008 (550 pages), ISBN 978-973-718-886-1(UPBuc. library);** **Impact:** the first monograph in Romania that presents (with hundreds of solved examples), in a systematic way, the numerical algorithms and statistical methods used for the primary treatment of data, and to evaluate the quality of the experimental (bio)chemical data. Course support (teaching textbook at U.P.Buc. (Bachelor BSC, MSC.) (U.P.Buc. library). . (in Romanian).
	**4.- Maria, G., Luţă, I., Numerical methods used for the math (kinetic) modeling and *in-silico* design of functionalized mesoporous structures for the controlled release of drugs in biologic fluids, Printech, Bucharest, 2015 (476 pages), ISBN 978-606-23-0443-0;** **Impact:** the first monograph in Romania that reviews (with numerous solved case studies), in a systematic way, the numerical algorithms and mathematical models (chemical kinetics, and/or diffusion transport) used to simulate the release of drugs from porous supports in biological fluids and ***in-silico*** design (based on mathematical models) of drug / functionalized micro-meso-porous support systems to obtain a programmable drug release (EU project – ZEOMED, 2011-2014) (U.P.Buc. library). . (in Romanian).
	**5.- Maria, G., Crişan, M., Maria, C., Parameters estimation of kinetic models for (bio)chemical processes, Printech, Bucharest, 2016 (528 pages), ISBN 978-606-23-0633-5;** **Impact:** the first monograph in Romania that reviews (with hundreds of solved examples), in a systematic way, the numerical algorithms and statistical methods used in the numerical treatment of experimental (bio)chemical data in order to identify an adequate kinetic model for a studied (bio)chemical process. Course support (teaching textbook at U.P.Buc. (Bachelor BSC, MSC.) (U.P.Buc. library). . (in Romanian). (in Romanian).
	**6.- Maria, G., A review of some novel concepts applied to modular modelling of genetic regulatory circuits, Juniper, Irvine (USA), 2017, (50 pages), ISBN 978-1-946628-03-9. https://juniperpublishers.com/ ebook-info.php;** **Impact:** the first monograph in the world that reviews (with some novel solved examples) the mathematical (kinetic) models used in the numerical simulation of cellular gene expression regulation (**GERM**), and of the genetic regulatory networks (GRC) responsible for the operons expression,, genetic switches, etc., in order to ***in-silico*** design genetically modified micro-organisms (**GMO**) for industrial or medical use. Support textbook for the "Metabolic engineering and bioinformatics " course at U.P.Buc. (MSc. In bioengineering) (library UPBuc., open-access).
	**7.- Maria, G., Deterministic modelling approach of metabolic processes in living cells - a still powerful tool for representing the metabolic process dynamics, Juniper, Irvine, California 91320, (USA), 2017, (50 pages), ISBN 978-1-946628-07-7(USA). https://juniperpublishers.com/ebook-info.php;** **Impact:** among the few monographs in the world that reviews (with novel examples solved by the author) the numerical methodology used to construct, on a deterministic basis, mathematical (kinetic) models used for the numerical simulation of some essential cellular metabolic processes, such as the central carbon metabolism (**CCM**), **GERM**, **GRC**, etc. All these (bio)chemical-mathematical tools are used for the ***in-silico*** design of **GMO**s for industrial or medical use. Support textbook for the "Metabolic engineering and bioinformatics " course at U.P.Buc. (MSc. In bioengineering) (library UPBuc., open-access).
	**8.- Maria, G., In-silico design of Genetic Modified Micro-organisms (GMO) of industrial use, by using Systems Biology and (Bio)Chemical Engineering tools, Juniper, Irvine, CA(USA), 2018, (100 pages), ISBN 978-1-946628-12-1(USA). https://juniperpublishers.com/ebook-info.php;** **Impact:** idem no.7.

	**9.- Maria, G., From residual biomass and inferior quality coal to the synthesis of methanol and then to hydrocarbons and gasoline – a Romanian project of high success, Juniper, Irvine, California(USA), 2018, (50 pages), ISBN 978-1-946628-16-9, https://juniperpublishers.com/ebook-info.php; Impact:** the only monograph that reviews a highly successful Romanian project from 1980-1995, namely the kinetic study of novel, avant-garde, non-conventional catalytic chemical processes that leading to the production - through methanol - of olefins (**MTO**), of aromatic hydrocarbons (**BTX**), or of synthetic gasoline (**MTG**) with high ON, by using cheap and/or renewable natural resources. The author was the key engineer who developed the kinetic models for these catalytic processes, further used for the technological design, construction and commissioning of an industrial plant at the Brazi Petrochemical Works (Ploiesti, ROU, 1985) to test these pioneering technologies in the world.
	**10.- Maria, G., Numerical algorithms to simplify the kinetic models of chemical and biochemical processes, Printech, Bucharest, 2019 (815 pages), ISBN 978-606-23-1010-3; Impact:** the first monograph in Romania that presents in a structured, extensive, and systematic way (with dozens of solved case studies) the numerical algorithms and statistical methods used to analyze the extended kinetic models of (bio)chemical processes in order to reduce them (by using "lumping" techniques " of chemical reactions/species, with preserving the reaction invariants) to simpler forms that can facilitate quick (bio)chemical engineering numerical analyses. (AR library, UPBuc. library). (in Romanian).
	**11.- Maria, G. (coordinator,95% of book), Gijiu, C.L., Dinculescu, D., Titica, M., Juncu, G., A review of unconventional technologies for capitalization of cheap natural resources (natural gas, lower coal), greenhouse gases (CO2) and renewable biomass for the production via methanol of a large number of high value-added chemicals and fuel by using technologies based on modern tools and concepts of chemical and biochemical engineering), Printech, Bucharest, 2020 (500 pages), ISBN 978-606-23-1143-8(AR library). Impact:** Among the few monographs in the world (and the only one in Romania) that reviews in a structured, and systematic way the main (non-)conventional technologies for capitalizing the cheap and/or renewable natural resources (e.g. low-grade coal, natural gas, CO2, municipal waste, biomass, etc.) for the production of a wide range of high-value chemical compounds. Several chapters are dedicated to the extensive description of a highly successful Romanian project that took place between 1980-1995, respectively the methanol conversion to hydrocarbons (**MTO, BTX, MTG**, book no. 9 from this list). This work is the result of the cumulated efforts of some members of the **IChB** Commission of the Romanian Academy, under the coordination of Prof. G. Maria. (AR, U.P.Buc. library). . (in Romanian).
	**12. Maria, G., About the school of (bio)chemical engineering and technology at the Polytechnic University of Bucharest, Printech, Bucharest, 2022 (800 pages), ISBN 978-606-23-1354-8. Impact: very high. The only monography in Romania that review, in a systematic and structured way, the history of the Romanian School of IChB. Thus, starting from the exceptional contribution of the founder Acad. Prof. Dr. Eng. Emilian Bratu, the book presents how the School of IChB at U.P.Buc evolved thanks to the contribution of the doctoral students trained by Prof. E. Bratu, and then by successive generations of teachers trained in the country but also abroad at the IChB departments of prestigious universities. Presentation is made in parallel with presenting the history and the evolution of IChB worldwide, of their concepts, principles, and work techniques. Thus, the successive adaptations of the study curriculum are presented, to keep up with the IChB high-level teaching at a world-wide level, as well as with the requirements of the Romanian economy which is in a continuous transformation to ensure sustainable technologies in a circular economy. To emphasize the value of the Romanian IChB school, the book also presents the most important industrial realizations of the members of the IChB Department of Polytechnic University of Bucharest, as well as some illustrative fundamental scientific contributions that belong to them. Special tribute chapters are dedicated to the founder of IChB in Romania, that is to Acad. Emilian Bratu, but also to those who made major contributions to the development of the IChB department, namely Prof. Raul Mihail (founder of the Romanian School of Chemical and Biological Reactors), Prof. Octavian Smigelschi (founder of the courses of optimization and automatic control of chemical processes), prof. Eli Ruckenstein (State University of New York at Buffalo; laureate of the USA National Medal of Science, 1998), Prof. Ovidiu Muntean (founder of the courses of biochemical and biological reactors), and others. (AR library, U.P.Buc. library).** . (in Romanian).
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	These math (models) tools are used i) for the *in-silico* design of GMOs, or ii) for deriving, with a high-precision, of optimal operating policies of bioreactors, by also accounting for the biomass evolution over long time intervals.

Papers in top ISI journals
selection from over 240 papers published in (bio-)chemical engineering journals and ISI conference proceedings (A complete list of Prof. Dr. GM can be found at his Research-Gate : Research-Gate = https://www.researchgate.net/profile/Gheorghe-Maria-2 an dat his web page from Googleschoolar

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III. IMAGES FROM HIS ACADEMIC LIFE (SELECTION)

Fig. 1A. Diploma and gold medal obtained at the 6th International Chemistry Olympiad for high school students (1974).

Fig.1B. Diploma of Excellence in Research granted by the Romanian Federation of Biomedical Engineering (2006).

Fig. 2A. [left] his PhD supervisor - Prof. Dr. Eng. Raul Mihail. Dissertation title: "Statistical estimation of parameters of mathematical models of chemical and biochemical processes" (1987); [center] Supervisor of his bachelor's thesis (chemical engineer diploma/licence) - Prof.dr.eng. Octavian Smigelschi. Dissertation title: "Mathematical Modeling and Optimization with using advanced numerical algorithms of a Multi-Cell Sugar Extractor (1979); [right] ing. G. Maria graduating as valedictorian the 5-years Faculty of Industrial Chemistry (1979).

Fig. 2B. Early activity at U.P.Buc. as a PhD student and teaching assistant (from 1980), then as a full lecturer (from 1990). Meeting of the group of Chemical Reactors in the laboratory in 1982, together with [from left] lecturer Iosif Nagy (now retired), the late assoc. Prof. C. Balaban, the late prof. Raul Mihail, dr. L.C. Tao (China), assistant G. Maria, professor O. Muntean (now retired), and the late lecturer M. Filipescu.

ACADEMIA ROMÂNĂ

DIPLOMA

În sesiunea din 30 mai 2019, Adunarea Generală a membrilor Academiei Române a ales, prin vot secret, pe domnul

GHEORGHE MARIA

Membru corespondent al Academiei Române

PREȘEDINTE
ACAD. IOAN-AUREL POP

SECRETAR GENERAL
ACAD. IOAN DUMITRACHE

BUCUREȘTI, 2019

Fig. 3. Corresponding member of the Romanian Academy diploma (2019).

Fig. 4. Some of the former PhD students of Prof. G. Maria in Chemical and Biochemical Engineering (2008-2023). [from left to right, top-then-bottom row]: 2011, Dragoș Nicolae ȘTEFAN (VEOLIA Water Techn. Co., Bucharest); 2013, Anca DAN (VTU Eng. S.A. Bucharest); 2013, Manuela Diana BUBOI (ENE after marriage)(Biotehnos S.A. Otopeni); 2014, Ionela LUȚĂ (TULIGA after marriage) (Siemens S.A. Bucharest); 2017, Hasan Hadi Salman KHWAYYIR (now lecturer with Najaf Technical College, Iraq); 2019, Constantin MUSCALU (Technology Consulting Manager at Accenture S.A. Bucharest); 2019, CRIȘAN Mara (Siemens S.A. Bucharest); 2020, Marina MIHALACHI (MUSCALU after marriage)(Petrodesign Bucharest) 2023; 2023, Laura RENEA (CERNENCU after marriage)(Lidas, Tulcea).

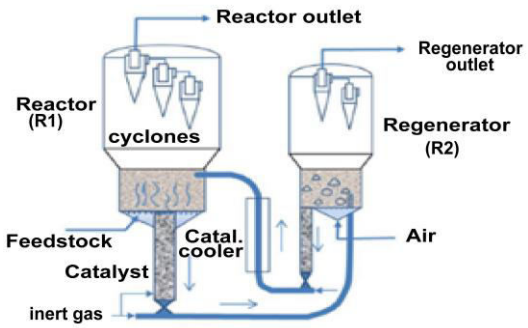


Fig. 5a. The industrial pilot plant for the conversion of methanol to olefins (MTO), or to synthetic gasoline (MTG), designed and put into service by Prof. G. Maria at the Brazi Petrochemical Works (Ploiesti, 1985)[5,6]

ACADEMIA REPUBLICII SOCIALISTE ROMÂNIA

ACADEMIA REPUBLICII SOCIALISTE ROMÂNIA

ACORDĂ

PREMIUL NICOLAE TECLU

TOV. MARIA GHEORGHE, G. MUSCA, GR. POP, ECATERINA POP, DOINA IVANESCU, N. IONESCU, ILEANA-JANETA IOSIF, M. RAUL, S. STRAJA, I. OLARU, I. GHEORGHE, LUCIA CREȚOIU, I. BELDEANU, GH. NICOLAE, RODICA BOERU

PENTRU Lucrarea "Catalizator și proces pentru conservarea metanolului la olefine"

DAT ÎN BUCUREȘTI LA 2 noiembrie 1985

PREȘEDINTE, Acad. Radu Voinea

SECRETAR, Prof. George Ciucu, membru corespondent

Nr. 20

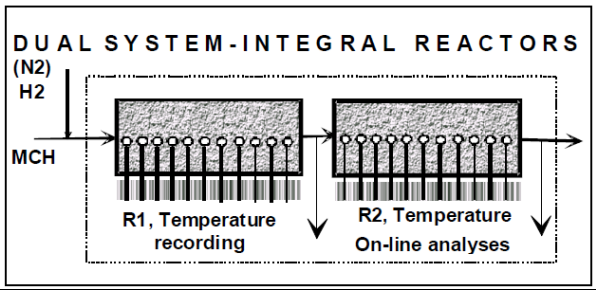
Fig. 6. The 'N. Teclu' award of the Romanian Academy granted to dr. G. Maria, for kinetic studies on the selective (catalytic) conversion of methanol to olefins (MTO) and to synthetic gasoline (MTG), and for the design, construction, commissioning, and on-line optimal control of this industrial plant from Brazi Petrochemical Works, Ploiesti (1985).

Fig. 5b. The industrial pilot plant for the conversion of methanol to olefins, and to synthetic gasoline (MTO/MTG) from the Brazi Petrochemical Works (Ploiesti, Romania), put into service in 1985 by a group of researchers and design engineers from IECB (ICECHIM) and IITPIC (Bucharest). The system of two fluid-bed catalytic reactors was technologically design by few members of the Chemical Reactors group from the Polytechnic University of Bucharest, led by Prof. Dr. Eng. Raul Mihail. A brief description of the project was made by the key research-design engineer of the project [Maria, G., From residual biomass and inferior quality coal to the synthesis of methanol and then to hydrocarbons and gasoline – a Romanian project of high success, Juniper, Irvine California USA, 2018, ISBN 978-1-946628-16-9; see book no. 9 above]. The detailed description was made by Dr. G. Maria, as being the key engineer of the project, namely the one who developed the kinetic models of the catalytic processes, and used them for the technological design of the industrial plant, that is the system of 2 catalytic reactors with continuous pneumatic transport between them [Maria et al., 2020] (book no. 11 from the above list).

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Fig. 7. Lecturer at ETH Zurich. [Top-left]: ETH Rectorate; [Upper right]: The previous dept. of Chemical Engineering of the ETH (Technische Chemie), located at Universitätstrasse 6 (1992-1997); [Bottom-left] Together with Prof. D.W.T. Rippin at ETH Zürich (1992) [Bottom right] ETH Polybahn (a-ETH city link).



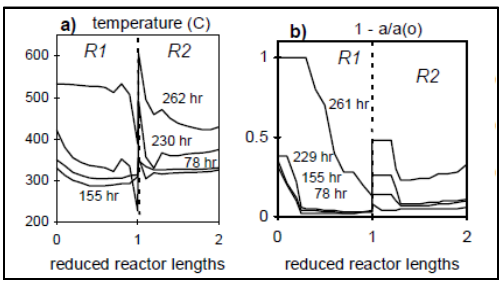


Fig. 8. The NEFF project. [Left] underdrawing of the pilot plant designed and commissioned by Prof. G. Maria at the Paul Scherrer Institut Villigen (Switzerland, 1995) for the chemical storage of hydrogen in MCH. [Right] Predictions for the long-time-on-stream of the temperature dynamics (a), and of the catalyst activity (b), in the series of reactors (R1-R2) used for the catalytic dehydrogenation of MCH to toluene (TOL) at 10 atm, 250-300 C with hydrogen release.

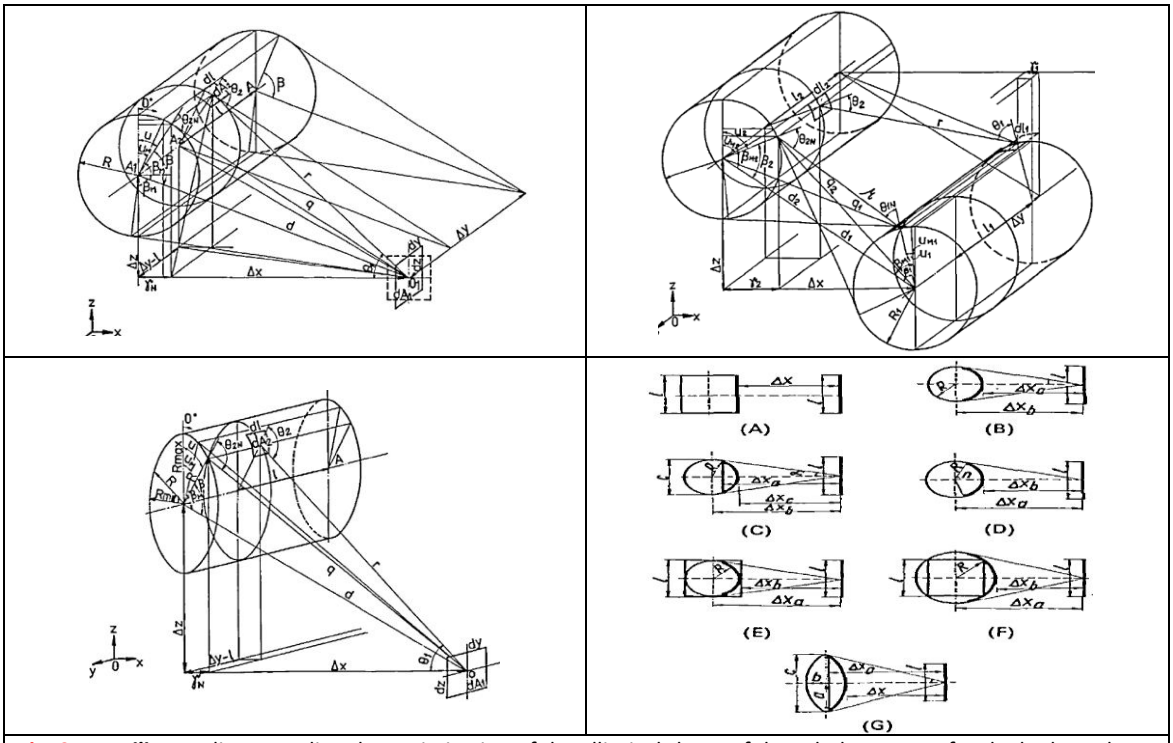


Fig. 9a. ***In-silico*** studies regarding the optimization of the elliptical shape of the tubular reactor for the hydrocarbons pyrolysis from Arpechim Pitești (ROU) Petrochemical Works (1980-1991). [Mihail and Maria, Int. Journal of Heat & Mass Transfer 26, 1783-1789 (1983). Doi:10.1016/S0017-9310(83)80149-5].

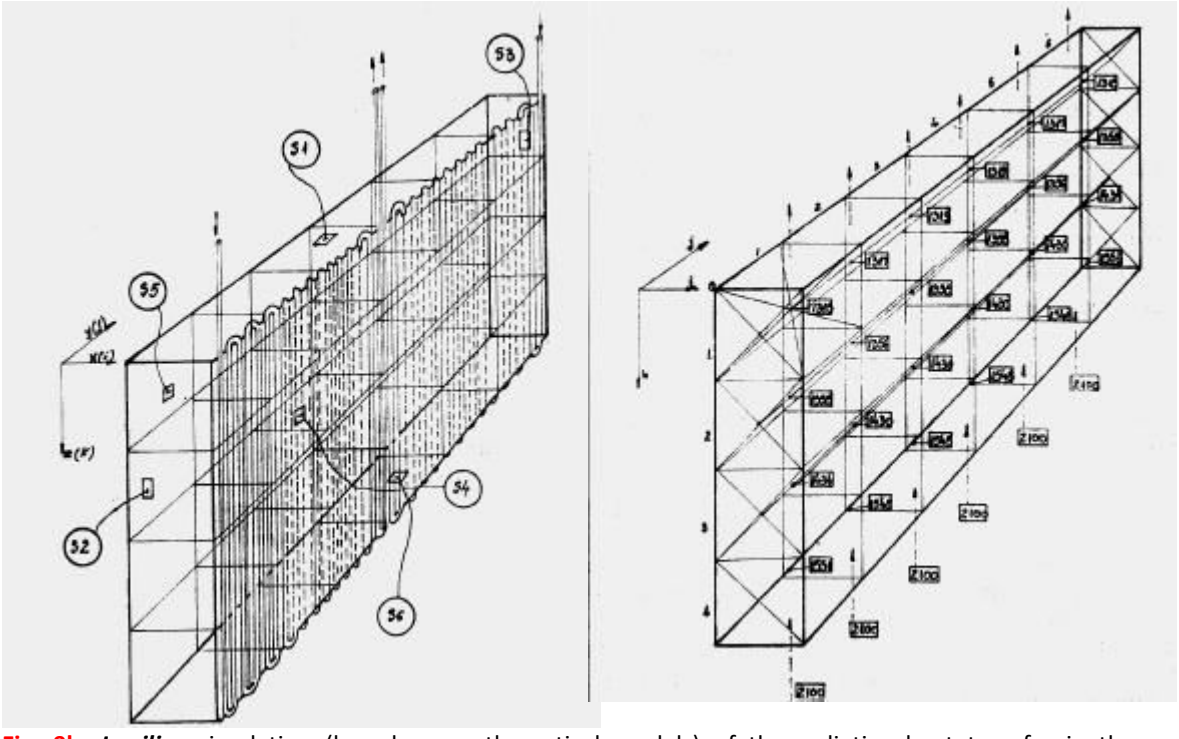


Fig. 9b. ***In-silico*** simulation (based on mathematical models) of the radiative heat transfer in the industrial pyrolysis furnace at Arpechim Pitesti Petrochemical Works (1979-1992), by using the "space zoning" method of [Hottel and Sarofim, Radiative transfer, McGraw, New York, 1967]. His relevant publications in this subject are [Mihail and Maria, , *Rev. Chimie (Bucharest)*, 32, 988-994 (1981); , *Rev. Chimie (Bucharest)*, 33, 157-161 (1982); Revue Roumaine de Chimie 32, 821-832 (1987)]

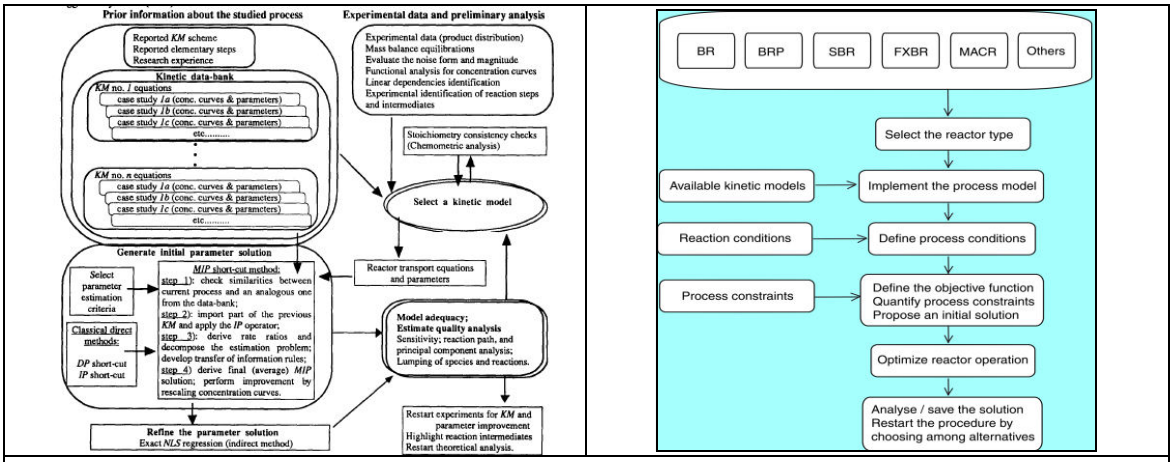


Fig. 10. [Left] The flow-chart of the KINEXP expert system for identifying the kinetic model of a (bio)chemical process, and for optimizing the related reactor by using direct (short-cut) numerical methods, and an original numerical algorithm to transfer information from kinetic data banks [7-9](Maria & Rippin, Comp. & Chem. Eng. 20, S587-S592, 1996). [Right] The flow-chart of the expert system developed by Prof. G. Maria to select and optimize the enzymatic reactor operation [7-9] (Maria, G., Comp. & Chem. Eng. 36(1), 325–341, 2012).

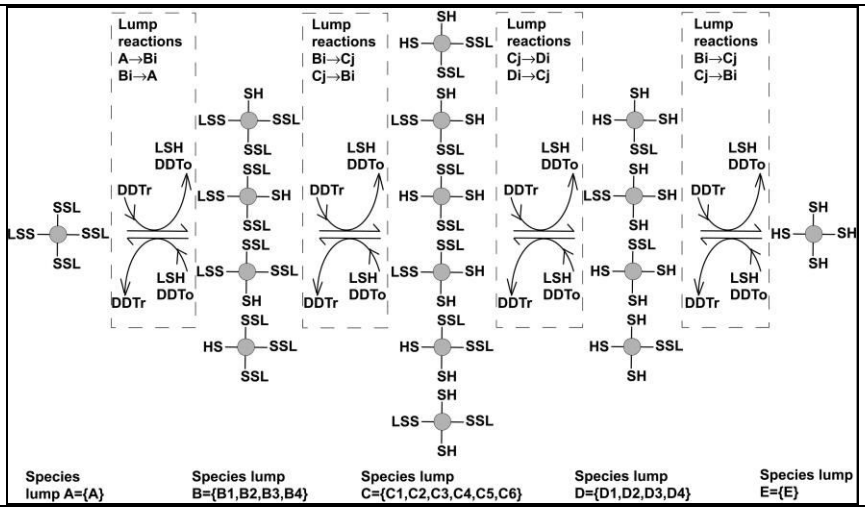


Fig. 11. The reaction pathway used by Prof. GM to simulate the dynamics of the chemically controlled release of drugs in human plasma from multivalent supports. The case study was also used to exemplify his proposed original numerical algorithms used for obtaining reduced kinetic models. These algorithms are based on the reaction invariants (Maria, G., Chem. Eng. Science 60, 1709-1723, 2005, doi:10.1016/j. ces.2004.11.009)

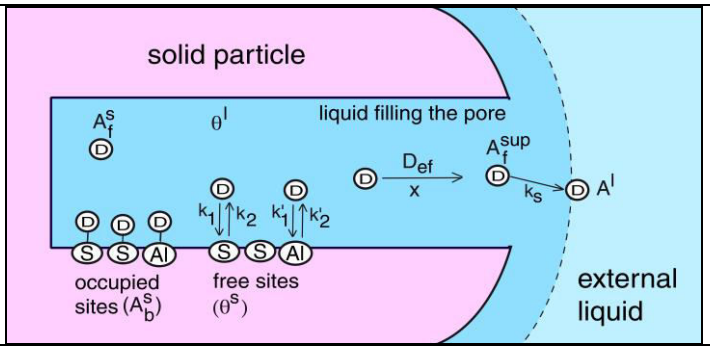


Fig. 12. Scheme of the math model used to simulate the dynamics of the chemically controlled release of drugs (A) from functionalized porous supports in biological fluids (book no. 4 from **Table 2**).

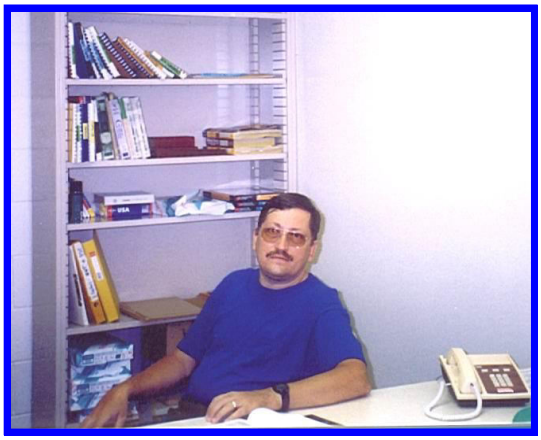
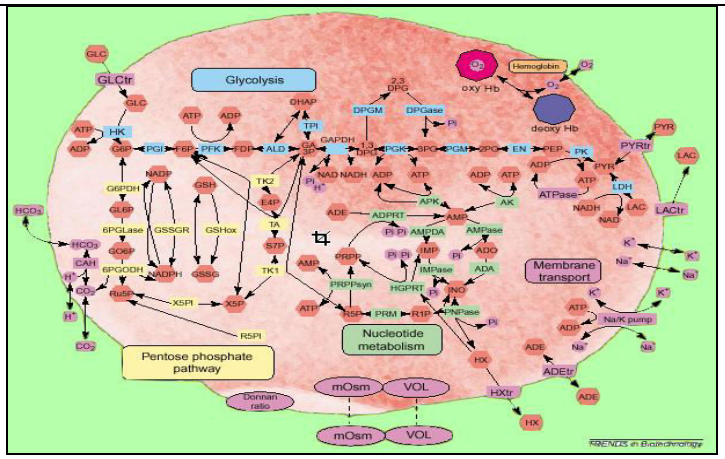


Fig. 13. Research activity at Texas A&M University, TAMU (College Station, USA)(2002-2003) with a NIH grant/stipendium. [Top-left] Faculty of Chemistry and Biochemistry of TAMU. [Top right] My office at TAMU. [Bottom]: Prof. Lindahl's working group dedicated to this NIH research project.



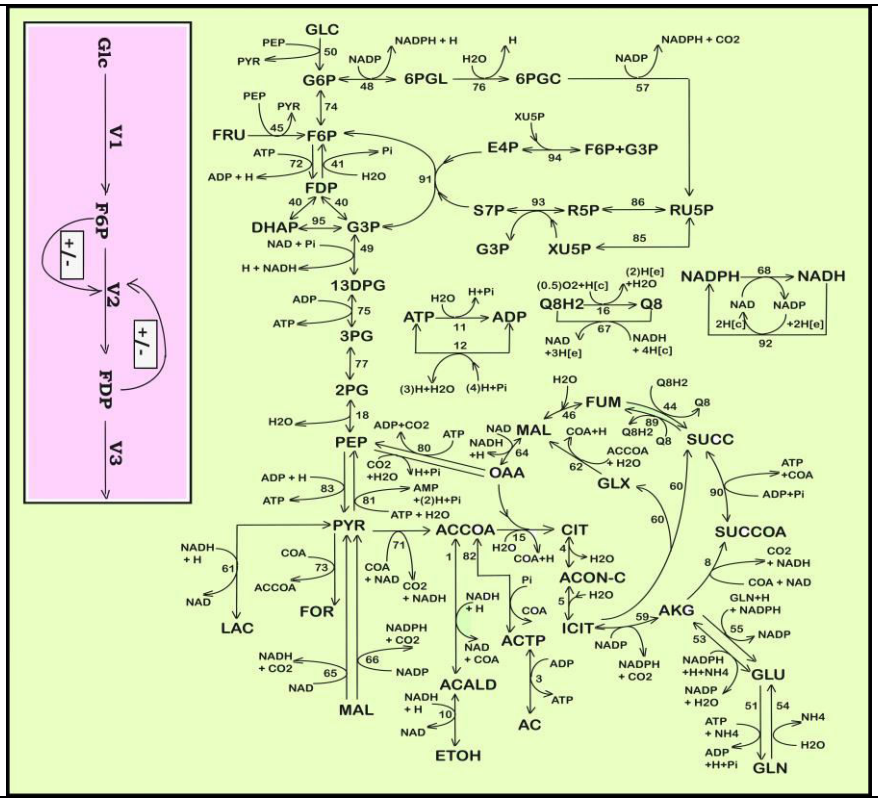
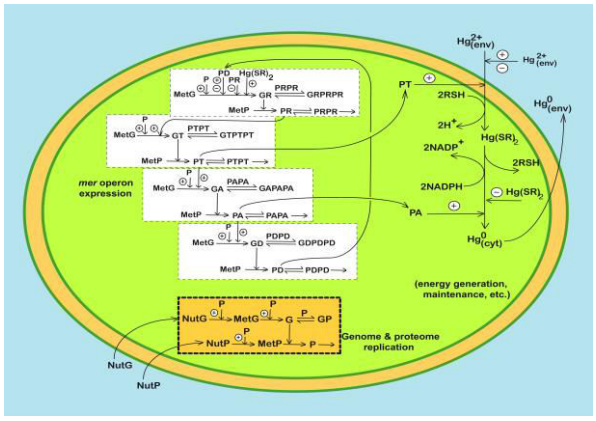


Fig. 14. [TOP] The reaction pathway framework used by prof. GM for the ***in-silico*** numerical simulation of CCM dynamics. [7-8] [DOWN] The reduced reaction pathway of CCM used for the ***in-silico*** design of genetically modified *E. coli* (**GMO**) to maximize the succinate production (Maria et al., **Chem. & Biochem. Eng. Q**. 25(4), 403-424, 2011)[7-8].



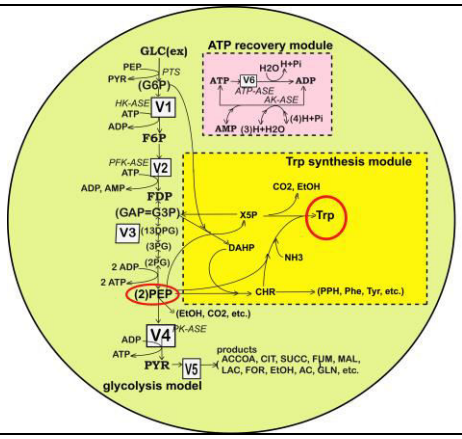


Fig. 15. [Left] Modular reaction pathway used by prof. GM to simulate the dynamics of the mercury operon expression in gram-negative bacteria (*E.coli*) - used for the ***in-silico*** design of cloned *E. coli* [7-9] (Maria & Luță, Comp. & Chem. Eng., 58, 98-115, 2013). [Right] Modular reduced reaction pathway used to simulate the glycolysis and the oscillating tryptophan (Trp) synthesis in *E.coli* (Maria, G., Frontiers in chemistry, vol. 8, pag. 526679, doi: 10.3389/fchem.2020.526679 2020). The hybrid, structured, modular dynamic model used for ***(i)*** the ***in-silico*** design of **GMO** E. coli to maximize the excretable Tryptophan (Trp) production [Maria, G., Computers & Chem. Eng., vol. 153, pp. 107450-107466 (2021). (IF=4.4), https://doi.org/10.1016/j.compchemeng.2021.107450], and for ***(ii)*** ***in-silico***, off-line optimization of the fed-batch bioreactor for Trp synthesis. [Maria, G., Renea, L., Bioengineering-Basel-MDPI, vol. 8 , no. 12, 210-247, 2021, IF = 6.1, https://doi.org/10.3390/bioengineering8120210]

Fig. 16. The front cover of the book published in 2020 by the Chemical and Biochemical Engineering Commission (**IChB**) within the Chemical Sciences section of the Romanian Academy (Maria, G. – Coordinator, 95% of the book, President of the Commission).

Fig. 17. Together with Prof. Jibin Sun and our wives, during a working visit to Tianjin Institute of Industrial Biotechnology, China (2010)

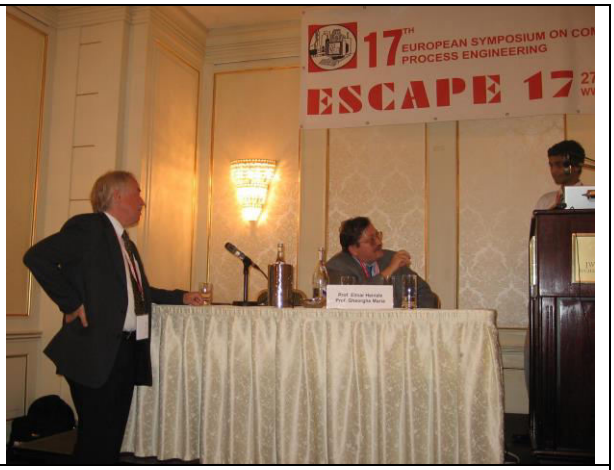


Fig. 18. Co-chairing together with Prof. Elmar Heinzle (Germany) the ESCAPE-17 international conference in Bucharest (2007)