



Prof. Dr. Ing. Gheorghe MARIA



TO PROFESSOR GHEORGHE MARIA ON THE OCCASION OF HIS 70th ANNIVERSARY – EXCELLENCY IN CHEMICAL AND BIOCHEMICAL ENGINEERING

Cristiana Luminita GIJU^{a,*}

^a Chemical and Biochemical Engineering Department, National University of Science and Technology POLITEHNICA Bucharest,
Str. G. Polizu 1–7, zip 011061, Bucharest, Roumania

Received April 3, 2025

I. SCIENTIFIC PROFILE

Prof. Dr. Ing. Gheorghe Maria from University Politehnica of Bucharest (**UPBuc.**), Department of Chemical and Biochemical Engineering is a valuable scientist in Roumania, being the successor and continuer of the Roumanian school of chemical, biochemical (enzymatic), biological reactors, and reaction engineering (founded by the late Prof. Raul Mihail), but also the creator of novel courses in the chemical engineer curricula at UPBuc.^{7,8a}

Prof. Maria was born on October 2, 1955 near Bucharest, in village Fundeni (Călărași county). He attended the Primary School in Bucharest, and then he followed secondary studies with “Gh. Lazăr” high school (1970–1974), in a specialized class in chemistry and math. He quickly became known for its original mathematical approach to solving complex chemistry problems. He has participated to numerous national chemistry and math school competitions (so-called Olympics), winning several prizes. Due to its outstanding results, on 1974 he was participated with the Roumanian team to the 6th International Chemistry Olympiad for high school students (11 participating European countries).^{1–3} At this famous traditional contest, GM won the gold medal by presenting ingenious math solutions to difficult chemical problems. Impressed by his success, the writer E. Seceleanu dedicated a chapter to him in his book.³

Following his exceptional achievements, on 1974 he was admitted to the UPBuc. without exam, at Fac. of Industrial Chemistry, where he chose major studies in Organic Chemistry, and Chemical Engineering. He graduated from UPBuc. in 1979, as valedictorian. After a short internship with chemical companies in Bucharest (1979–1982), he was hired (1982) as a senior research engineer by **ICECHIM** – Chemical and Biochemical Energetics Inst. Bucharest (**IECB**), being in charge with modelling the kinetics of (bio)catalytic processes, and technological design of industrial plants.

Over 1981–1987 he performed PhD studies under the supervision of prof. Raul Mihail, entitled “*Statistical estimation of (bio)chemical process models parameters*”, by approaching case studies related to the kinetic modelling of a large number (more than 40) of catalytic (bio)chemical processes mostly by using the IECB experimental data.

Gheorghe Maria has had an exceptional career as a chemical engineer, developed over four decades, gaining experience from all sides of the profession: production, research, and teaching. On 1990 Gheorghe Maria was hired by UPBuc. as a lecturer. Over the next two decades he was hired by top universities in

* Corresponding author: luminita_gijiu@yahoo.com

temporary positions, or invited to make short summer internships (see the below section). Thus over (1992–1998) he was **Assistant Professor** (Oberassistent Klass 18) with **ETH Zürich** (Switzerland), being involved in teaching (MSc/PhD), but also in research projects dealing with: a) chemical reactor math-model-based design, optimization, and risk analysis; b) (bio)chemical kinetics modelling; c) development of novel statistical estimation rules in chemical kinetics; d) large-scale prospective research projects with industrial realizations, below described.

On 1998 Gheorghe Maria return to Roumania and completed all the university degrees up to the present one of Prof. Dr. Ing. (1999), with UPBuc., Lab. of biochemical reactors.

Over 2002–2003 GM was an invited Senior Res. Scientist with **Texas A&M University**, Dept. of Chemistry and Cell Biology (College Station, USA), to be part of a NIH project on bioinformatics, that is math-modelling / numerical simulation of gene expression regulatory modules (**GERM**), and of genetic regulatory circuits (**GRC**) dynamics in living cells, aiming to design genetically modified micro-organisms (**GMO**) of industrial / medical use.

International cooperation. After 1990, prof. Gheorghe Maria was invited as a *visiting professor* to participate to numerous (beyond 20) scientific research projects with prestigious universities worldwide (section II.2.2). Thus, he carried out short (3 months) research stages in i) Canada at Queen's Univ. Kingston, (1994); ii) in Germany at: Univ. des Saarlandes (1999); TU Erlangen (2000); TU Braunschweig (2006, DFG project); TU Hamburg (2009); iii) at Univ. Porto, Portugal (1999, NATO project); iv) in France at EP Grenoble (1998); v) in China at Tianjin U. (2010); vi) Texas A&M Univ. (USA; NIH fellow 2002–2003).

In short, the approached topics during his stays abroad are related to i) modelling / optimization of catalytic chemical reactors; ii) bioinformatics applications dealing with in-silico design (using numerical simulators) of GMOs for industrial/medical use (books B8–10); iii) quantitative (math-model-based) risk analysis of catalytic chemical reactors (book B2).^{4,7,8b}

The time spent with these research groups allowed him not only to exchange / develop valuable scientific ideas, but also to establish strong cooperations in its research areas (chemical kinetics / reactors, bioinformatics), thus enabling exchange of students, access to international grants, joint publications, etc. The significant number (ca. 30) of invited lectures presented at esteemed universities reflects the value of his world-wide recognized contributions to his specific field. Among the *invited lectures* are to be mentioned: ETH Zurich 1992–1997, RWTH Aachen 2006, U. Leeds 1996, U. Liverpool 1996, EPF Lausanne 1993–1996, U. Zagreb 2007, BASF Germany 1995, TU Erlangen 2000, TU Hamburg 2009, TU Saarbrücken 1999, TU Braunschweig 2006; in USA (Princeton U. 1994, Texas A&M U. 2002–2003), etc.

His **research area** includes a wide range of “classic” engineering fields, that is: chemical, biochemical, and biological reactors (math model-based design, optimization, control); modelling (bio)chemical kinetics (books B3,5,9,10,11); numerical engineering analysis; theoretical and applied statistics (books B1,3,5); numerical optimization methods (book B1,5,10), etc, but also “modern border fields“, namely: quantitative (model-based) risk analysis of chemical reactors (book B2); bioinformatics (math modelling and simulation of cell metabolic process dynamics, of **GERM**, **GRC**, books B6–8; B13), and math modelling of the controlled drug release in biological fluids (book B4).

The theoretical (fundamental) scientific works in the above mentioned topics, as well as the industrial practical achievements of prof. Gheorghe Maria are impressive.^{4,6,7,8a,8b,10} Its **high scientific productivity** includes over 250 papers in ISI journals and intl. Conferences proc. (from which 55 in Q1–Q2 top journals), most of them as principal author, 16 ISBN books (8 in RO, and 8 in USA); 5 teaching ISBN books at UPBuc., and 12 ISBN book chapters (see below selection), with a H-index of 23 (googlescholar), and 24 (RG-scopus), and I-10 of 67, with above 2200 citations.

Based on his research experience gained as a key-investigator to a large number of research projects with various EU and US universities, prof. Gheorghe Maria has promoted in the chemical engineering education and research in Roumania (at UPBuc.) advanced directions, compatible with those developed in the EU. Thus, as a professor with UPBuc., Gheorghe Maria was highly appreciated as being a dynamic element in the perpetual renewal of the Faculty curricula, and its adaptation to the requirements of a modern European education and performance. Thus, GM was the architect of **new courses in the curricula** of the chemical engineer at UPBuc, namely: i) “Risk and safety quantitative assessment of chemical processes/reactors” (BSc/MSc); ii) “Metabolic engineering of living cells and bioinformatics” (MSc); iii) “Statistical treatment of experimental chemical data” (BSc,MSc); iv) “Biochemical

engineering”^{7,8a,8b,10} While prof. Raul Mihail (1920–1985) was the creator of the Roumanian School of Chemical, Reactors, by publishing the first course in Roumania of “Chemical Reactors” (1971), and the late prof. Ovidiu Muntean was the creator of the Roumanian School of Biochemical, and Biological Reactors, prof. Gheorghe Maria was one of the valuable continuators of their work, making a bridge over the years by developing a modern school of (bio)chemical reactors and bioinformatics at UPBuc., by promoting it both at theoretical and applied levels, within numerous research projects, and publications,^{7,8a,8b,10} but especially through materialized innovative applications in the chemical industry (see below). **Teaching activity.** As a full habil. Prof. (1999–present) with Dept. of Chemical and Biochemical Engineering (IChB) from **UPBuc.**, Prof. GM is the successor, promoter, and developer of the Roumanian 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 of chemical engineering (book B12)).^{7,8a,b,10} In short, prof. Gheorghe Maria teach/supervised BSc, MSc courses/projects in Chemical and Biochemical Engineering (1980–present) at UPBuc. Between 2006–2011, he was in charge with implementing and supervising the MSc. in Biochemical Engineering and Bioengineering at UPBuc. Between 1980–present he supervised more than **50** undergraduate (BSc.) projects, over **22** MSc. Diss., and of **12** PhD students (10 finalized and 2 in progress) in his topics at UPBuc. At UPBuc. Prof. Gheorghe Maria teach the following courses, some being novel courses introduced by Gheorghe Maria: **i)** Reactors and chemical and biochemical reactions engineering (BSC); **ii)** Numerical and statistical methods for treatment of experimental (bio)chemical data, and to estimate the parameters of (bio)chemical process math models (novel since 1997); **iii)** Quantitative analysis (based on mathematical models) of the operating risk of chemical processes and reactors. Numerical simulation of the consequences of a chemical accident (fire, explosion, toxic substances releases) (novel since 2006); **iv)** Biochemical Engineering (novel, since 2015); **v)** Metabolic Engineering and Bioinformatics (novel, since 2004).

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. Gheorghe Maria promoted in the field of chemical engineering education in Roumania (at UPBuc.) various avant-garde courses and research directions, comparable with those developed in the EU, related to bioinformatics, chemical reactor operation safety, and others (see the above list). Prof. Gheorghe Maria wrote and published the related teaching manuals/text-books (books B1–B13). Through all these books, prof. Gheorghe Maria had and has a significant impact on the science and practice of the chemical and biochemical reactions engineering and reactors in Roumania and world-wide.

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. The use of deterministic, modular, structured, hybrid dynamic models, linking the cell-level state variables to the bioreactor macroscopic-level state variables for **1)** *in-silico* design of **GMOs**, and **2)** a more accurate optimization of industrial bioreactors operation, with a higher degree of detail (no. of cell/bioreactor state variables). The cell-level kinetic models include the essential modules of the central carbon metabolism (**CCM**) beside the module concerning the synthesis of the target metabolite (of interest). *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: mathematical 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. Gheorghe Maria has made fundamental theoretical contributions in several frontier fields, namely “systems biology” and “synthetic biology”, “bioinformatics”, “computational biology”. The essential one, consists in the introduction and validation of the novel “**mechanistic silicon cell concept**”, materialized in a novel math (kinetic) modelling framework **WCVV** of cell metabolic processes (referring to the “whole-cell, variable-volume”, of isotonic growing cells)[books B6–B8,B13]. The **WCVV** is particularly suitable to characterize the regulatory properties of self-regulated gene (**GERM**) / operon expression, and of genetic regulatory circuits (**GRC**), but also the **CCM**, metabolic processes, in a holistic approach. Prof. Gheorghe Maria proved that the novel **WCVV** holistic kinetic modelling framework of cell metabolic processes (in an isotonic growing cell) is superior compared to the classical (default) **WCCV** (“whole-cell, constant-volume”) kinetic modelling framework which offers **distorted, and wrong** simulation results [paper P34]. This fundamental theoretical contribution applies to the *in-silico* (math model based) dynamic simulation of cell metabolic processes. In particular, the novel **WCVV** it is very suitable to characterize the regulatory properties of self-regulated gene (**GERM**) / operon expression, and of genetic regulatory circuits (**GRC**) [B6–B8,B13]. Math modeling of the drug release kinetics in biological fluids for *in-silico* design of optimized controlled (programmable) release systems [book B4].

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 [books B9,B11].

II.2. The results of his research activity

The results of his research activity are materialized in: ^{7,8a,8b,10}

Publication productivity

Major industrial realizations

Published Theoretical contributions (basic / fundamental research)

Summary of his publishing activity

The numerous theoretical (fundamental) but also practical (industrial) achievements of prof. Gheorghe Maria are also reflected through a rich publishing activity. His main publications include the followings (see his below publicationlist):^{7,8a,8b,10}

- 8 ISBN books in Roumanian,
- 8 ISBN books in English in the USA,
- 5 ISBN university textbooks (U.P.Buc.),
- 12 book chapters with ISBN abroad,
- main author of above 170 papers in ISI esteemed journals (over 50 in top IChB publications)
- (co-)author of above 85 papers in international scientific conferences.

All the above books, with the exception of the university textbooks (written in collaboration) have prof. Gheorghe Maria as sole author, or as main author (coordinator). His publications are well cited (**Hirsch index 23/24, I10 index 67**, with over **2200 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 Roumanian classification system (MEdC-OMs-2011).

Major industrial achievements of Prof. GM include the followings realizations:

1) *Design and scale-up the MTO/MTG industrial plant*. Between 1981–1991, dr. Gheorghe Maria 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, Roumania)^{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 B 9, B 11).

In this context, must be underlined the remarkable, exceptionally valuable, and pioneering studies conducted by prof. Gheorghe Maria 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. Gheorghe Maria in top **ICH** journals, and they represented the foundation for the design and construction of the demonstrative industrial plant for the above mentioned processes at the Brazi Petrochemical Works (Ploiesti, Roumania), activities in which prof. Gheorghe Maria had a major / key contribution [books B9,B11]. The MTO/MTG industrial plant (Fig. 1a–b), with the characteristics presented in [books B9,B11], includes two chemical catalytic 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. At that time (1980–1985), this industrial plant was the first in the world to test MTO/MTG processes by using this novel un-conventional 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) [book B11]. Later, industrial MTO/MTP plants were built by UOP/Hydro co. in Germany and in China, but using different technologies [book B11].

By using this industrial plant, and the experimental data provided by IECB, prof. Gheorghe Maria 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) [books B9, B11].

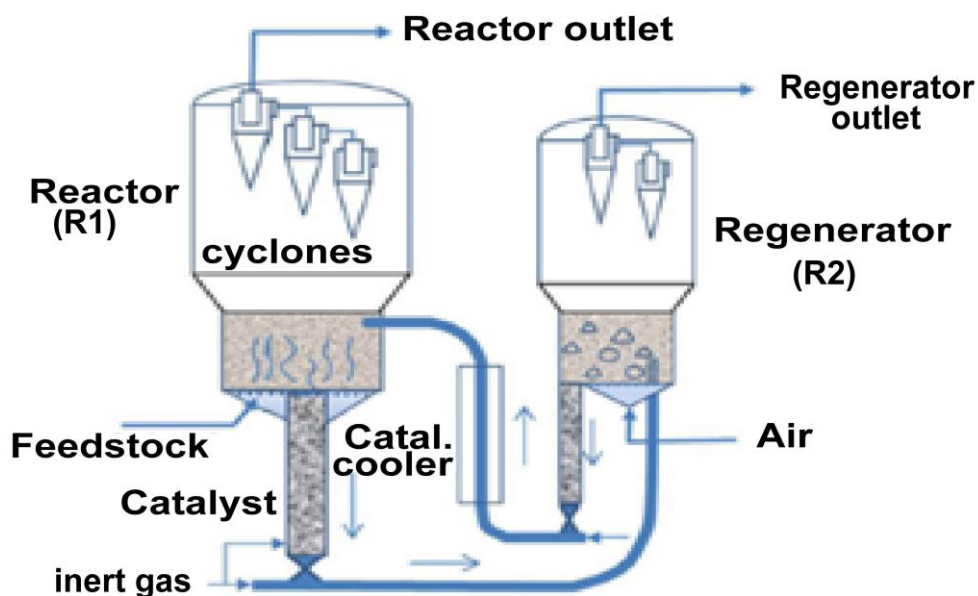


Fig. 1a – The industrial pilot plant for the conversion of methanol to olefins (MTO), or to synthetic gasoline (MTG), design and put into service by prof. Gheorghe Maria at the Brazi Petrochemical Works (Ploiesti, 1985) [books B9,B11].



Fig. 1b – The industrial pilot plant for the conversion of methanol to olefins, and to synthetic gasoline (MTO/MTG) from the Brazi Petrochemical Works (Ploiesti, Roumania), 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 the few members of the Chemical Reactors group from the UPBuc., led by prof. Raul Mihail. A brief description of the project was made by the key research-design engineer of the project Gheorghe Maria [books B9, B11]. Dr. Gheorghe Maria was one of the key engineer of the project, who developed the kinetic models of the catalytic processes, used them for the technological design of the industrial plant, that is a system of 2 catalytic fluidized-bed reactors with continuous pneumatic transport between them [books B9, B11].

For such an exceptional achievement, prof. Gheorghe Maria received (as a research/key design engineer, and part of the research/design team involved in this project of tremendous importance) the “Nicolae Teclu” Award of the Roumanian Academy in 1985 (Fig. 2).

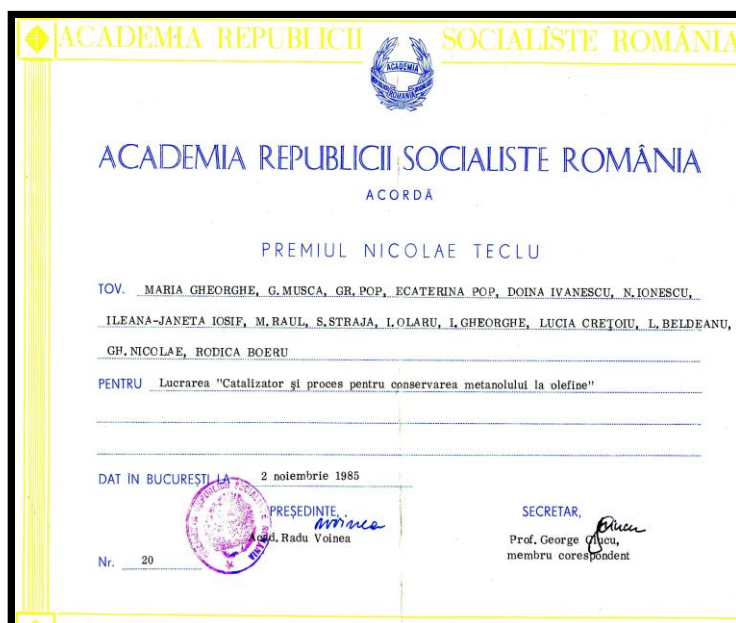


Fig. 2 – The “N. Teclu” award of the Roumanian Academy granted to dr. Gheorghe Maria, for kinetic studies on the selective (catalytic) conversion of methanol to olefins (MTO) and to synthetic gasoline (MTG), and for the design, construction, commissioning, and on-line optimal control of this industrial plant at Brazi Petrochemical Works, Ploiesti (1985–1992).

2) Pilot plant for the chemical storage of energy (via hydrogen) and its transport at long-distances.

In 1992, dr. Gheorghe Maria chose to accept an invitation and he came to Switzerland to work as an Assistant Professor (Oberassistent Klasse 18) with the Polytechnic University ETH Zürich, in the "Process Systems Engineering" group of the late prof. David WT Rippin (Chemical Engineering Dept.). Here, prof. Gheorghe Maria was involved in teaching activities (supervising, or co-supervising PhD/MSc students). But also, he actively participated as a key [investigator/researcher] to the materialization of several important research projects of the group, in the (bio)chemical engineering area.

One of these industrial-scale projects (NEFF) concerns the technological design and commissioning by prof. Gheorghe Maria of a medium-sized, fully automated pilot plant consisting of a system of two fixed-bed catalytic reactors linked in series (Fig. 3), 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). Then, the MCH is 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. Gheorghe Maria 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 [paper P5].

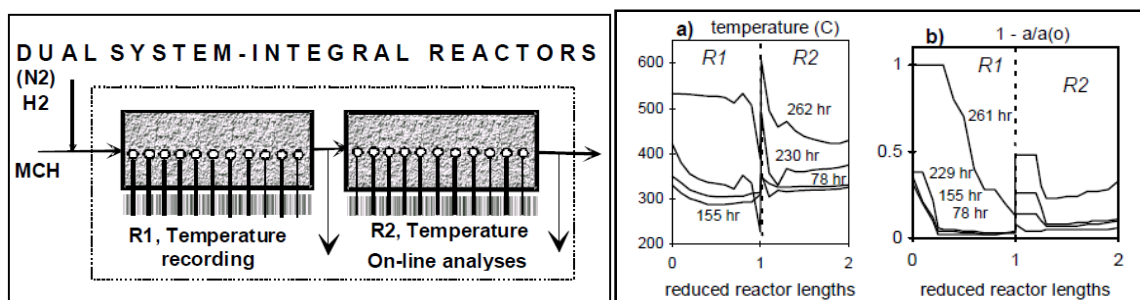


Fig. 3 – The NEFF project. [Left] the scheme of the pilot plant design and commissioned by prof. Gheorghe Maria at the Paul Scherrer Institut Villigen (Switzerland, 1995) for the chemical storage of hydrogen in MCH. [Right] Predictions for the long-time-on-stream of the temperature dynamics (a), and of the catalyst activity (b), in the series of two reactors (R1-R2) used for the catalytic dehydrogenation of MCH to toluene (TOL) at 10 atm, 250–300 C with hydrogen release, or for the catalytic hydrogenation of TOL to MCH at 220 C and 30 atm.

3) In-silico optimization of the safe operation of some high-risk chemical catalytic reactors. Another research project where prof. Gheorghe Maria 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 pharma industry, operated by Novartis (Basel, Switzerland, 1992–1997).

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. Gheorghe Maria 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 inherent presence of random fluctuations of the control parameters. See his top publications [papers P46, P47, P48, P49].

4) Optimization of an existing industrial plant. Right from the first years of his career, dr. Gheorghe Maria was involved in research topics aiming at optimize the existing industrial reactors in Roumania. One of these applications refers to the optimization of the hydrocarbons pyrolysis reactor at Arpechim Pitești Petrochemical Works, Roumania (1980–1991).

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 (Figs. 4a–b). See his works [P50–P52, P60, P61].

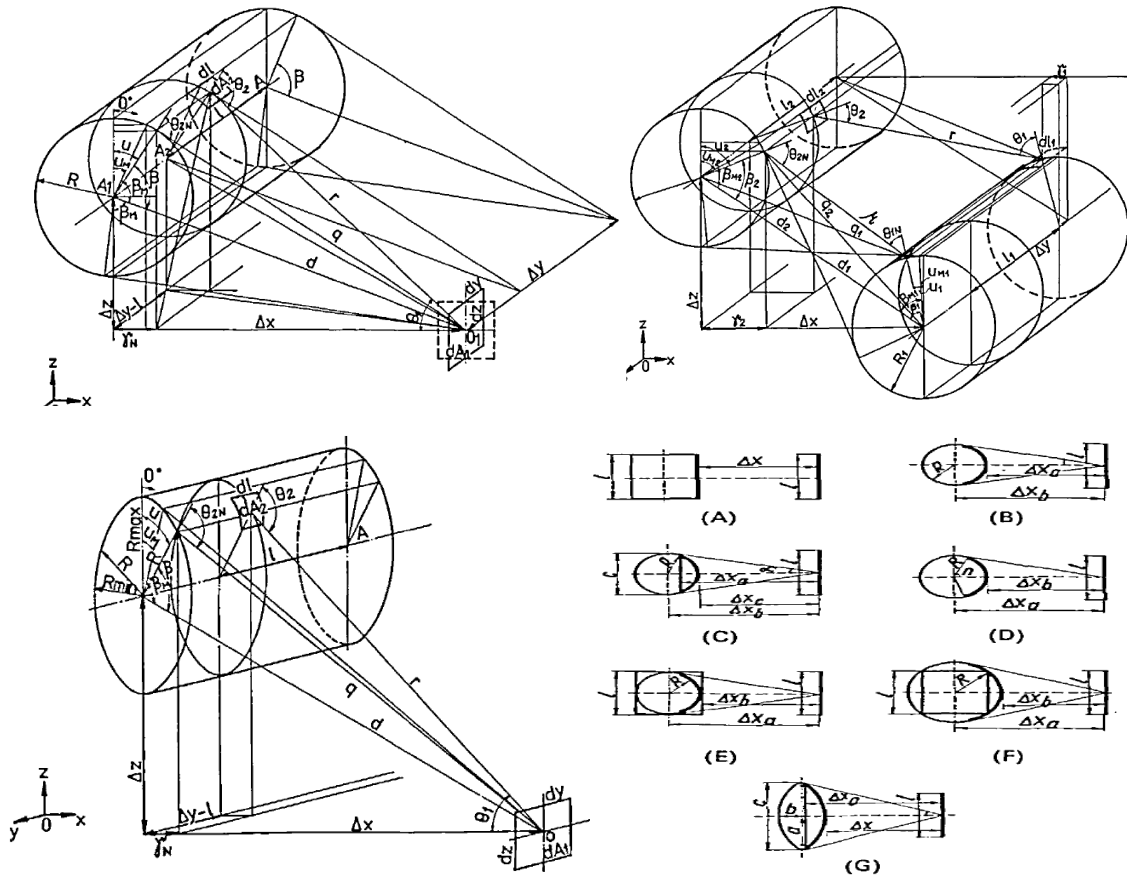


Fig. 4a – *In-silico* studies regarding the optimization of the elliptical shape of the tubular reactor for the hydrocarbons pyrolysis from Arpechim Pitestî (ROU) Petrochemical Works (1980–1991) [P52].

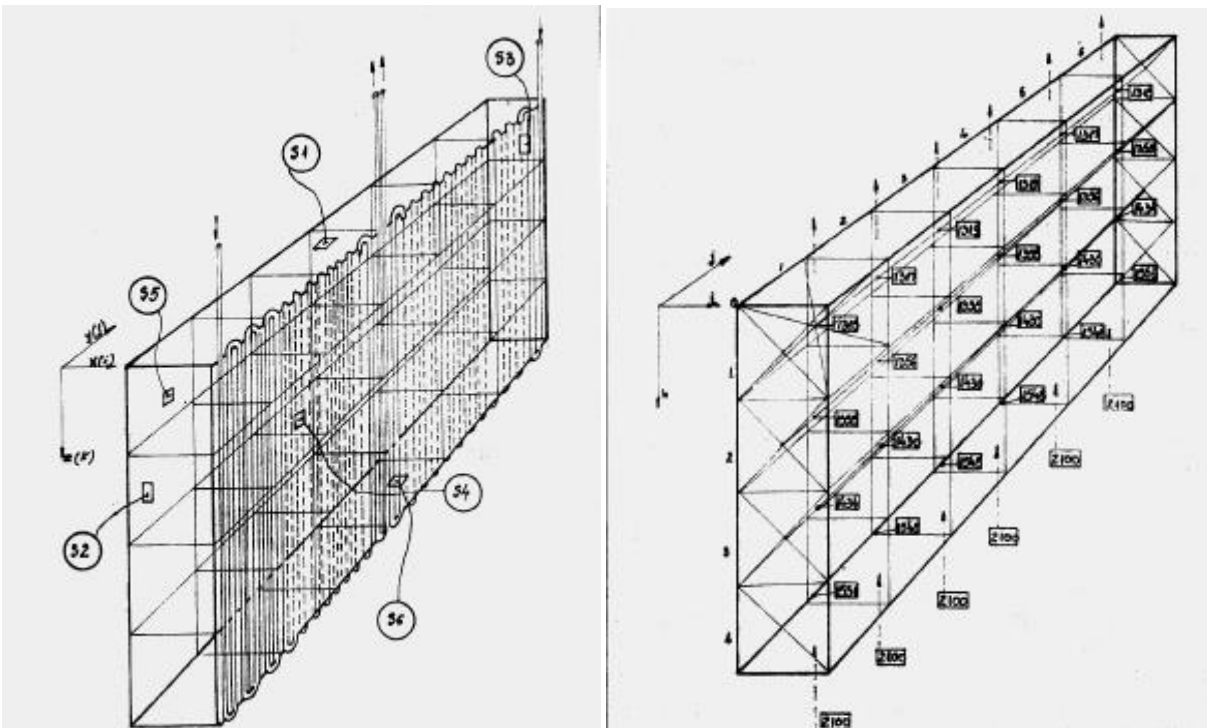


Fig. 4b – *In-silico* simulation (based on mathematical models) of the radiative heat transfer in the industrial pyrolysis furnace at Arpechim Pitestî Petrochemical Works (1979–1992), by using the “space zoning” method of [Hottel and Sarofim, Radiative transfer, McGraw, New York, 1967]. Prof. Gheorghe Maria relevant publications in this subject are [P50–P52,P60,P61].

Theoretical (fundamental) contributions with major impact

T1. 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. Proposal of a very large number (over 40)^{7,8a,8b,10} of complex kinetic models for various catalytic, processes (chemical, enzymatic, and cellular biological) [books B6–B9,B11,B13].

ii. Mathematical modeling, numerical simulation, and in-silico, off-line determination of the optimal operating policies of chemical, biochemical and biological reactors of all types. 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).^{7,8a,8b,10} Development of an expert system KINEXP 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. 5, right). Application of advanced (multi-objective, Pareto-front) numerical optimization rules, with a large number of original elements [P32,P33]. Their contributions are exemplified for a very large number of case studies: (i) enzymatic conversion of glucose to fructose [P53,P41]; (ii) enzymatic conversion of fructose to mannitol [P19,P25,P27,P29,P30]; (iii) synthesis of tryptophan in biological reactors [P26,P28]; (iv) mercury removal by modified E. Coli in trickle-bed bioreactors [P12]; (v) monoclonal antibodies production by using a hybridoma cell culture in a FBR bioreactor [P21,p54] (vi) succinate synthesis in a batch bioreactor [P55], etc.

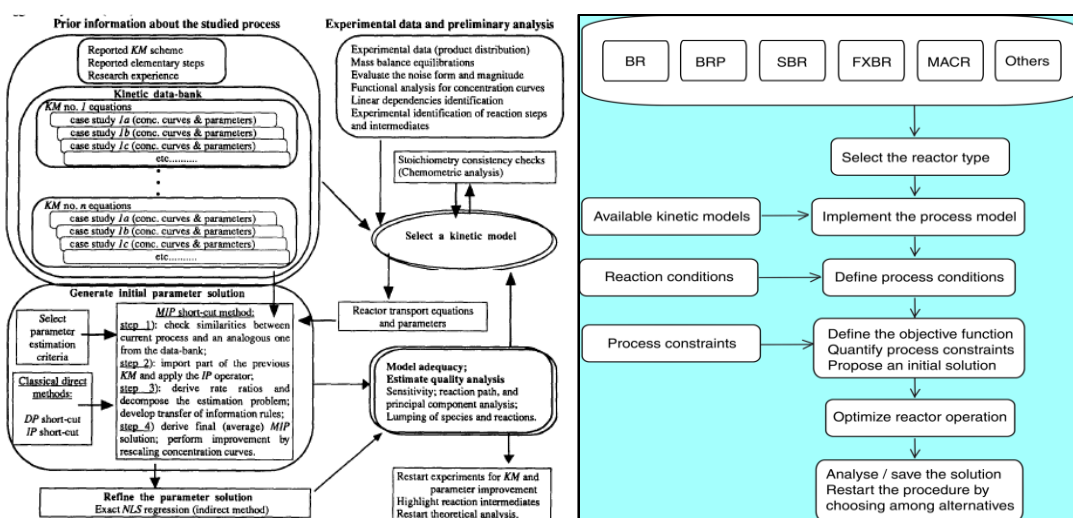


Fig. 5 – [Left] The flow-chart of the KINEXP expert system for identifying the kinetic model of a (bio)chemical process, and for optimizing the related reactor by using direct (short-cut) numerical methods, and an original numerical algorithm to transfer information from kinetic data banks [papers P4,P6,P18]. [Right] The flow-chart of the expert system developed by prof. Gheorghe Maria to select and optimize the enzymatic reactor operation [paper P11].

T2. Quantitative in-silico analysis of the thermal runaway risk of a chemical reactor (where exothermic fast 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.^{7,8a,8b,10}

b. in-silico assessment of the chemical process technological risk and of their environmental impact, by using math 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. Gheorghe Maria wrote and published the first monography / teaching book in Roumania (2007) in this field [book B2];

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 (P56,P57).

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.^{7,8a,8b,10}

T3. 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. 6–7, book B4).

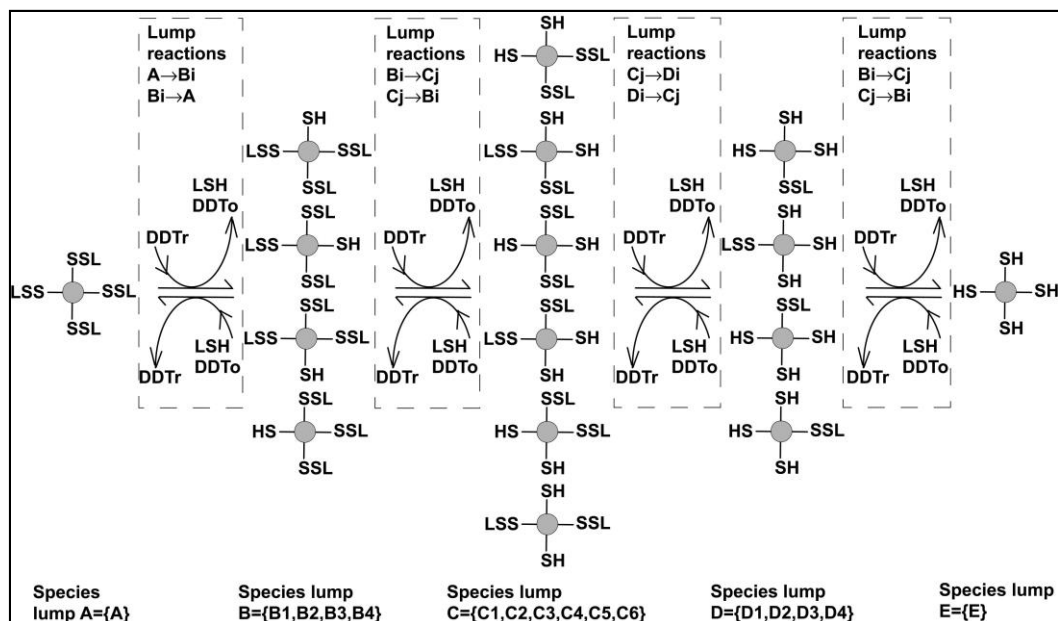


Fig. 6 – The reaction pathway used by prof. Gheorghe Maria to simulate the dynamics of the chemically controlled release of drugs in human plasma from multivalent supports. The case study was also used to exemplify his proposed original numerical algorithms used for obtaining reduced kinetic models. These algorithms are based on the reaction invariants [P17].

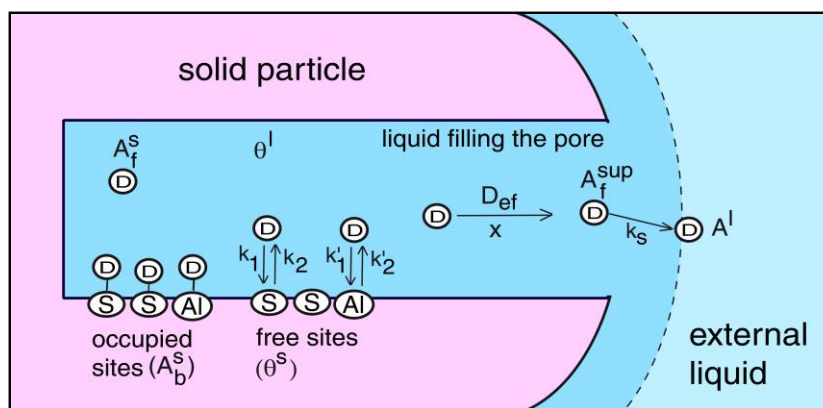


Fig. 7 – Scheme of the math model used to simulate the dynamics of the chemically controlled release of drugs (A) from functionalized porous supports in biological fluids (book B4).

T4Bioinformatics. In 2002, prof. Gheorghe Maria 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: 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. Gheorghe Maria 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. His published contributions in this topic (books B6-B8,B13) refer to:

(i). Proposing the novel “mechanistic silicon cell concept”, materialized in a novel math (kinetic) modelling framework **WCVV** of cell metabolic processes (referring to the “whole-cell, variable-volume”, of isotonic growing cells able to maintain intracellular homeostasis while growing auto-catalytically on environmental nutrients present in variable amounts). The **WCVV** is particularly suitable to characterize the regulatory properties of self-regulated gene (**GERM**) / operon expression, and of genetic regulatory circuits (**GRC**), but also the central carbon metabolism (**CCM**) (Fig. 8), metabolic processes, in a holistic approach. The **WCVV** is also very suitable to develop dynamic math hybrid **hybrid MCSMD models (structured, of modular construction and deterministic)** (with continuous variables, based on the cell metabolic reaction mechanisms) linking the key-species of the central carbon metabolism (**CCM** Fig. 8), of individual gene expressions (**GERM**), and of the genetic regulatory circuits (**GRC**) responsible for regulating the essential cellular metabolic syntheses, to the macro-molecular state-variables of the studied bioreactor. These dynamic hybrid bioreactor models are then used for 1) *in-silico* design of **GMOs** used in industrial biosynthesis, medicine, etc. [books B6–B8,B13]. Among them it is worth mentioning: a) *in-silico* design of **GMO *E.coli*** in order to maximize the mercury removal from wastewaters (Fig. 9, left); b) *in-silico* design of **GMO-modified *E.coli*** in order to maximize the tryptophan production (Fig. 9, right); iii) *in-silico* design of **GMO modified *E.coli*** to maximize the succinate production (Fig. 8), and others. 2) *in-silico*, off-line optimization of the bioreactor operating policy with a higher precision, and with a higher degree of detail (no. Of simulated cell.reactor species).

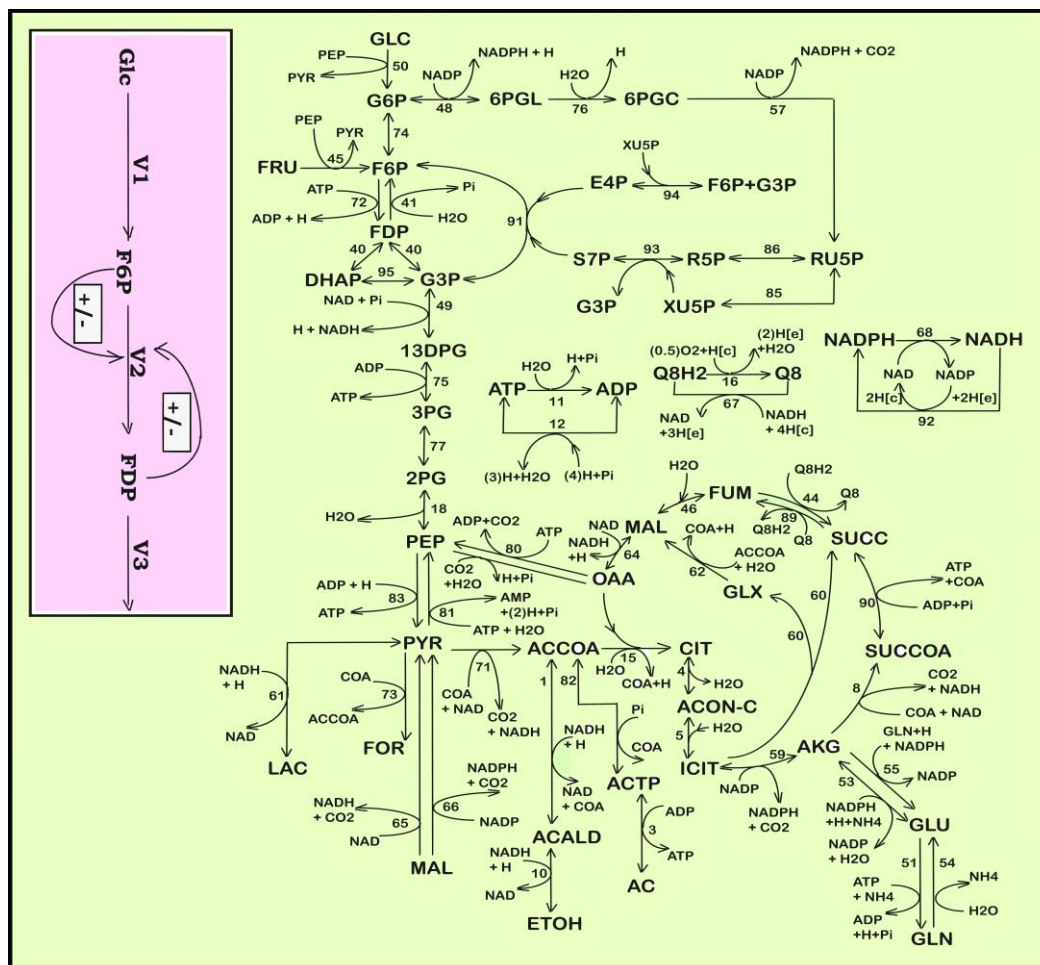


Fig. 8 –The reduced reaction pathway of **CCM** used for the *in-silico* design of genetically modified *E. coli* (**GMO**) to maximize the succinate production [papers P55,P26].

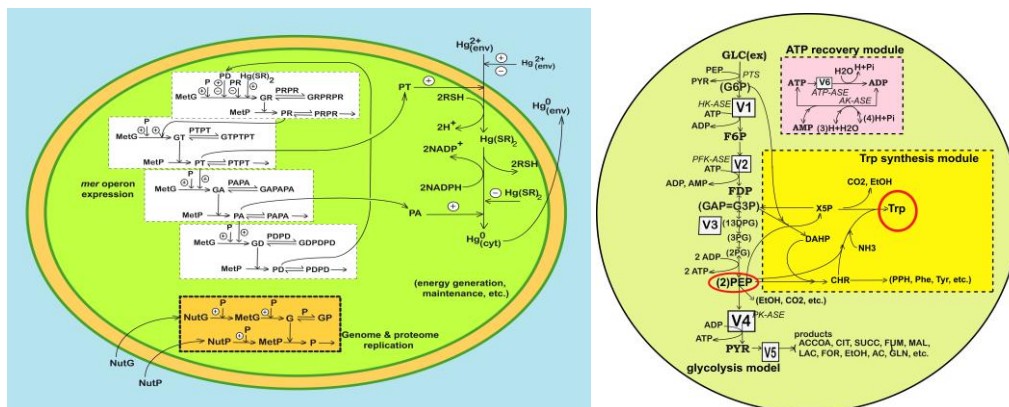


Fig. 9 – [Left] Modular reaction pathway used by Gheorghe Maria to simulate the dynamics of the mercury operon expression in gram-negative bacteria (*E.coli*) – used for the *in-silico* design of cloned *E. coli* [P12]. [Right] Modular reduced reaction pathway used to simulate the glycolysis and the oscillating tryptophan (Trp) synthesis in *E. coli* [P15,P16,P20,P23,P24,P26,P28]. The hybrid, structured, modular dynamic model was used for (i) the *in-silico* design of **GMO** *E. coli* to maximize the excretable Tryptophan (Trp) production [P26], and for (ii) *in-silico*, off-line optimization of the fed-batch bioreactor for Trp synthesis [P28].

In brief, the proposed “**Mechanistic silicon cell**” novel concept and the novel **WCVV math modelling framework** considerably improves the kinetic models of cell **CCM/GRC** processes, as followings (Fig. 10):

- Fundamental theoretical contributions for the *In-silico* (math model based) dynamic simulation of cell metabolic processes. In particular, Gheorghe Maria introduced and validated the novel “mechanistic silicon cell concept”, materialized in a novel math (kinetic) modelling framework WCVV of the cell metabolic processes (referring to the “whole-cell, variable-volume”, of isotonic growing cells able to maintain intracellular homeostasis while growing auto-catalytically on environmental nutrients present in variable amounts) [see their hypotheses in books B6–B8,B13]. The WCVV is particularly suitable to characterize the regulatory properties of self-regulated individual gene expression (GERM), and of genetic regulatory circuits (GRC) (*e.g.* genetic switches, genetic amplifiers, operon expression, etc.)
- He also proved that the novel WCVV kinetic modelling framework of cell processes is superior compared to the classical (default) WCCV (“whole-cell, constant-volume” like) kinetic modelling framework, the latter offering distorted, and wrong simulation results [P58].
- Use of instant cell dilution “ D_i ” in the cell species mass balances of WCVV models instead of the “default” average dilution $D_m = \ln(2)/(\text{cell cycle})$, or even its omission in the classical WCCV models [books B6–B8,B13].
- Applications of WCVV *hybrid* (structured, of modular construction, and deterministic) MCSMD models to *in-silico* design of GMOs, and for a more accurate optimization of industrial bioreactors operation, with a higher degree of detail (no. of cell/bioreactor state variables).
- Being very suitable to simulate GERM/GRC of living cells, the WCVV was used to develop a math “LIBRARY” (Fig. 11) including “template” kinetic models of the main GERM types. This library is useful to build-up dynamic models of GRCs (genetic regulatory circuits), useful for *in-silico* design of genetically modified micro-organisms (GMOs). The use of the novel WCVV math modelling framework to define novel quantitative performance indices (P.I.-s) to better characterize the regulation efficiency of individual GERM-s related to external perturbations [dynamic (“pulse-like”), or stationary (“step-like”)]. The use of the GERM library and their P.I.-s to propose a “building-blocks” strategy and rules to connect GERM-s to build-up GRC when designing desirable GMO-s. Some of these GERM-s structures were experimentally validated [books B6–8,B13].
- The GERM – LIBRARY (Fig. 11) was also used to *in-silico* study the cell self-regulation properties, impossible to be highlighted by using classical cell WCCV models.
- In other words, this huge contribution presents a holistic “closed loop” approach that facilitate the control of the *in vitro* through the *in-silico* development of dynamic models for living cell systems, by deriving *deterministic, modular, structured, hybrid* cell kinetic models (MCSMD), with continuous variables, linking the cell state-variables to the bioreactor ones.
- Such complex WCVV kinetic models are used in engineering evaluations for various purposes: 1) to simulate the essential parts of the central carbon metabolism (CCM), such as: glycolysis, TCA cycle, ATP

recovery system, or various other cell systems, such as: the mercury operon expression; Tryptophan TRP operon expression; succinate synthesis, etc., aiming to *in-silico* design of GMO-; 2) to simulate and/or design various genetic regulatory circuits (GRC); examples include: genetic switches (biosensors), genetic amplifiers, operons expression. 3) to *in-silico*, off-line derive optimal operating policies of bioreactors, with a higher precision and degree of detail. [books B6–B8,B13].

A novel math (kinetic) modelling framework of the cell metabolic process. That is [**WCVV** = "whole-cell, holistic approach of isotonic, variable volume, growing cell systems"]. It is very appropriate to simulate the dynamics of the self-regulation of individual gene expression modules (**GERM**), and of the genetic regulatory circuits / networks (**GRC**).

Isotonic ($\pi=ct.$), isothermal cell system
 $RT/\pi = 1/\sum C_j = \text{const.}$ **Pfeffers' law**

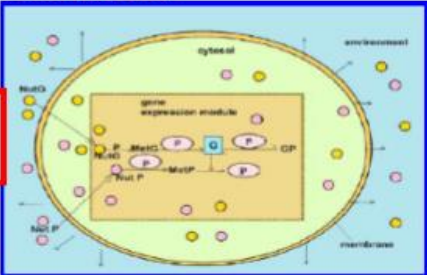
$$\frac{dC_j}{dt} = \frac{d}{dt} \left(\frac{n_j}{V} \right) = \frac{1}{V} \frac{dn_j}{dt} - \frac{n_j}{V} \frac{dV}{dt} = \frac{1}{V} \frac{dn_j}{dt} - DC_j = h_j(C, k, t)$$

Use of instant cell dilution "Di" in the **WCVV** models, instead of the "default" use of the average "Dm" !!!

$$D_m = \frac{d(\ln(V))}{dt} = \ln(2)/t_c$$

$$D_i = \frac{1}{V} \frac{dV}{dt} = \left(\frac{RT}{\pi} \right)^{n_s} \sum_j \left(\frac{1}{V} \frac{dn_j}{dt} \right)$$

Simplest (lumped) reaction Pathway of a GERM



- Isothermal, isotonic, open system, negligible gradients
- Quasi-constant osmotic pressure (inner and outer cell)
- Semi-permeable membrane, following the cell growing dynamics ; (t_c = cell cycle)
- Include all cell components at a certain degree of detail
- Account for holistic cell properties (ballast effect, constant osmotic pressure , π , variable volume, cell cycle)

Estimation of model parameters (k) and of un-observable species conc. (C_A):

- Solving the kinetic model steady-state (QSS) form, using the known species homeostatic concentrations
- Max. QSS recovering rates of the cell system state-variables (key-species conc.) after dynamic perturbations
- Max.(QSS) species conc. sensitivities vs. stationary perturbations from environment
- Min. transition times between two QSS-s after a stationary perturbation
- Max. regulatory effectiveness of GRC (P.I.-s) of GRC with maximizing the QSS stability strength

Fig. 10 – The essential concepts / relationship and hypotheses of the **WCVV** modelling framework.

Notations: C_j = species "j" concentration; n_j = species "j" number of moles (copynumbers); V = cell (cytosol) volume; R = universal gas constant; T = absolute temperature; π = osmotic pressure; t = time; D_i = instant cell dilution rate; D_m = average cell dilution rate; n_s = number of considered species (individually, or lumped) in the cell model [books B6–8,B13].

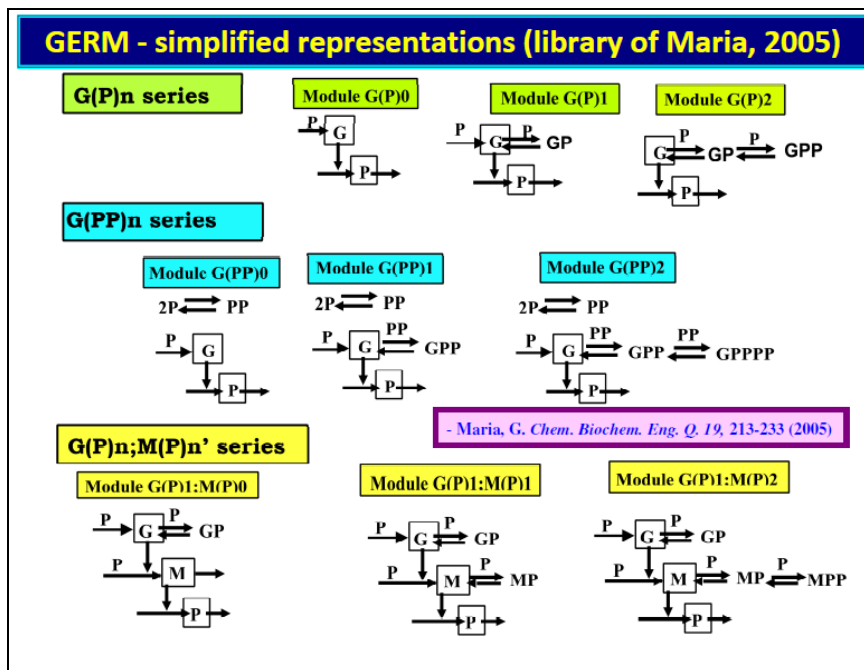


Fig. 11 – The "LIBRARY" of lumped modular models of gene expression regulatory modules (GERMs) developed by Maria [books B6–B8,B13].

The library of Fig. 11 includes, in a template form, the kinetic models corresponding to simplified representations of a generic gene expression G/P regulatory module (**GERM**), assimilated with formal mutual catalytic actions of G and P. The horizontal arrows indicate reactions, while the vertical arrows indicate catalytic actions. The absence of a substrate or product indicates an assumed concentration invariance of these species. Notations: G = gene encoding P; M = mRNA.

[Up-row]. Simplified representation of the gene expression models corresponding to **[G(P)n]** regulatory module types. The transcriptional factor is the protein P itself, the self-regulation over the transcription and translation steps being lumped together. To improve the system homeostasis stability and self-regulation, despite perturbations in nutrients Nut*, and metabolites Met*, or of internal cell changes, a very rapid buffering reaction $G + P \rightleftharpoons GP(\text{inactive})$ has been added, once time, or several times.

[Middle-row]. Simplified representation of the gene expression model corresponding to a **[G(PP)n]** regulatory module types. The transcriptional factor is the dimmer PP. The other observations from the top-row also apply here.

[Down-row]. Simplified representation of the gene expression model corresponding to **[G(P)1; M(PP)n]** regulatory module types. The models account for the cascade control of the expression via the separate transcription and translation steps.

Notations: G = DNA gene encoding P; M = mRNA; P,PP = allosteric effectors of the transcription / translation. The other observations from the top-row also apply here.

T5. Contributions to basic numerical calculations and statistical algorithms.

Prof. Gheorghe Maria has developed new numerical algorithms for solving non-linear optimization/estimation problems used to solve difficult problems related to identifying (bio)chemical kinetic models, and to optimizing (bio)chemical or biological reactors. The most important numerical algorithms developed and published by Gheorghe Maria are the followings:

MMA, MMAMI [P3,P8,P7] – 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. Gheorghe 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. Gheorghe 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. Biotechnology (China) (2010).

CPEMR [P59] – 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;

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) (caption Fig. 5, 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. 6 and book B10).

MIP [P4,P6,P18]– 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..

RSA [book B10] – an original statistical test for determining the redundant part of a kinetic (bio)chemical model.

GHSM [P2] – A Numerical Procedure for Solving Nonlinear Mathematical Models by Using a Generalized Search Interval Halving Method.

DSC-MIP [P56,P57] A combined experimental method (DSC calorimetry), with a numerical algorithm (MIP) for identifying the global chemical kinetic math models.

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 (intrinsic) kinetic model (64 reversible reactions, and 16 species) used to simulate the dynamics of chemically controlled release of drugs from a **[multivalent dendrimeric support]**. This extended kinetic model was finally reduced (by using this lumping technique

(book B10) to an “apparent (global)” model with only 4 reversible reactions that include 5 groups of conformational isomers, with rate constants estimable from the experimental data [P17] (Fig. 6). 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).

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); *ROMPHYSICHEM 15-th Intl. Conf. of Physical Chemistry*, 11–13 Sept., 2013, Bucharest; *13th Conf. Academic Days* Timișoara, June 13–14, 2013; *ESCAPE-17 (European Symp. Computer Aided Proc. Eng.)*, 27–30 May 2007, Bucharest, etc.

More than 30 invited 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 Saarbrücken (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. Babeș-Bolyai Cluj (2013); Inst. Of Biochemistry of the Roumanian 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, Timișoara (RO), 26 May 2011; 15-th ROMPHYSICHEM, Intl. Conf. Physical Chemistry, 11–13 September, 2013, Bucharest; 12-th ELSEDIMIA 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 Saarbrücken (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 Roumania 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 Brașov, RO); iii) Co-chairman Intl. conf. ESCAPE-17/CAPE, Bucharest, 27 May 2007; 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* (Croatia); 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 Roumanian Chemical Engineering Society*; 6) *ECOTERRA Journal of Environmental Research and Protection* (Roumanian 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* (Roumanian 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];
- 1985, “Nicolae Teclu” Award of the Roumanian 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, Roumania) [5,6,7–9] (Figs. 1a–b, Fig. 2);
- 2006, Diploma of Excellence in Research, granted by the Roumanian Federation of Biomedical Engineering;
- 2010–2021, above **20** awards from the Roumanian Research Agency UEFISCDI, for top papers published in top journals (Q1–Q2);
- 2019, unanimously elected as Corresponding Member of the Roumanian Academy (Chemical Sciences section);
- 2020, designated as President of the Chemical and Biochemical Engineering Commission (**IChB**), within the Chemical Sciences section of the Roumanian Academy (Fig. 12);
- tribute papers and booklets dedicated to prof. Gheorghe Maria;⁴⁻⁷
- The book B10 from the below list was nominated (position 1 out of 3 proposals) for the “G. Moisil” award of the Roumanian Academy (2023);

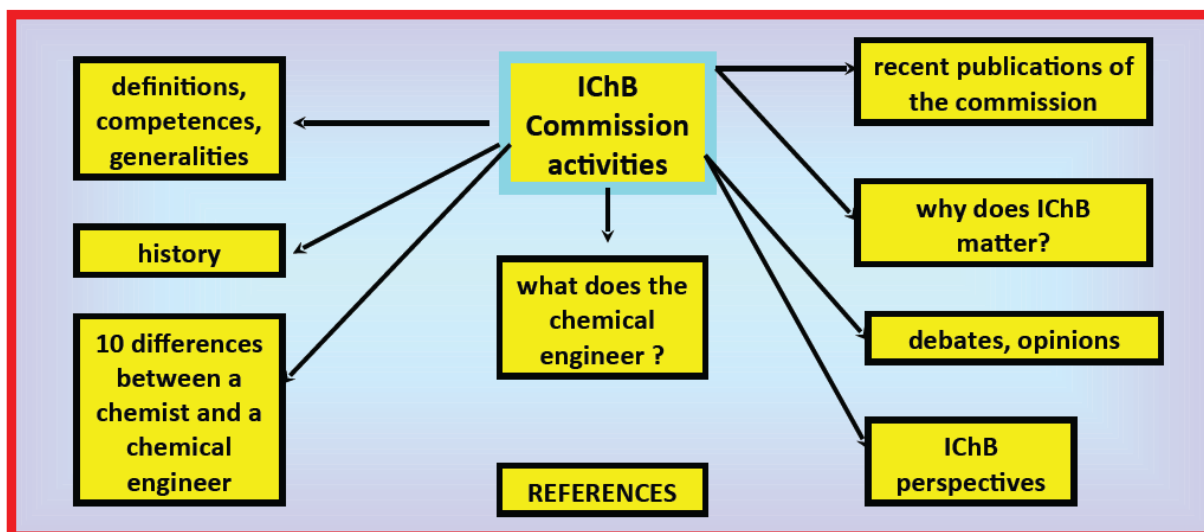


Fig. 12 – Activities of the **Chemical & Biochemical Engineering Commission (IChB) of the Roumanian Academy**. Details on its web page (in Roumanian) = <https://acad.ro/institutia/comisiile.html?21>

ACTIVITY WITHIN THE ROUMANIAN ACADEMY

Head of a Specialized commission. From January 2020, prof. Gheorghe Maria is the president of the Chemical and Biochemical Engineering Commission (**IChB**) within the Chemical Sciences section of the Roumanian 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** in EU, and 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 Roumania. See Fig. 12 for the commission activities, and its web-page. Two of such works dealing with the future **IChB** in the EU and in Roumania were published in 2020 by the **IChB-AR** Commission, respectively books B11–B12 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 Roumanian Academy, and **Chemical and Biochemical Engineering Quarterly** (edited by the Chemistry and Chemical Engineering Society of Croatia).

Some activities as President of the Chemical & Biochemical Engineering Commission (IChB) of Roumanian Academy (Fig. 12):

- The commission WEB-page = <https://acad.ro/institutia/comisiile.html?21>
- (17 Oct. 2024): Commemorative session. Tribute to Acad. Prof. Emilian BRATU – the founder of the Roumanian School of Chemical Engineering (120 yrs from his birth).
- Published 2 books of high impact, by the IChB commission, namely books B11, B12 of the below list.

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 Roumanian Society of Chemical Engineering, of the Roumanian Society of Chemistry, of the Roumanian Society of Bioengineering and Biotechnology, of the Alumni association of former DAAD scholars (Germany), of the National Society of Environmental Science and Engineering (Roumania), 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);
 - Several DAAD research grants in Germany: Univ Saarlandes (1999); TU Hamburg (2009).

PUBLISHED WORK (SELECTION)

The almost complete list of publications by Prof. GM can be found at his personal web page from ResearchGate = <https://www.researchgate.net/profile/Gheorghe-Maria-2>
Or at his web-page from Google Scholar.

ISBN books

Selection from 16 books published in Roumania and USA; 5 ISBN university textbooks; 12 chapters of ISBN books in English. Libraries where the books are available: AR = Roumanian Academy; UPBuc. = Polytechnic University of Bucharest.

B1	Iordache, O., Maria, G. (60%), Corbu, S., Statistical modeling and the estimation of parameters for chemical processes, Roumanian Academy (RA) publ., Bucharest, 1991, 240 pages (ISBN 973-27-0195-1) (AR; UPBuc. library).
B2	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)
B3	Maria, G., The statistical treatment and correlation of experimental (bio)chemical data. DStatistical distributions and estimators, Printech, Bucharest, 2008 (550 pages), ISBN 978-973-718-886-1(UPBuc. library)

B4	Maria, G., Luță, I., Numerical methods used for the math (kinetic) modeling and <i>in-silico</i> 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
B5	Maria, G., Crișan, M., Maria, C., Parameters estimation of kinetic models for (bio)chemical processes, Printech, Bucharest, 2016 (528 pages), ISBN 978-606-23-0633-5
B6	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
B7	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
B8	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
B9	Maria, G., From residual biomass and inferior quality coal to the synthesis of methanol and then to hydrocarbons and gasoline – a Roumanian project of high success, Juniper, Irvine, California(USA), 2018, (50 pages), ISBN 978-1-946628-16-9, https://juniperpublishers.com/ebook-info.php
B10	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
B11	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 (CO ₂) 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).
B12	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.
B13	Maria, G., Hybrid modular kinetic models linking cell-scale structured CCM reaction pathways to bioreactor macro-scale state variables. Applications for solving bioengineering problems, Juniper, Irvine, CA(USA) 2023, (300 pages), ISBN 978-1-946628-24-4.

Papers in top ISI journals

Selection from about 250 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> and at his web page from Google Scholar

- P1. Mihail, R., Straja, S., Maria, G., Musca, G., Pop, G., Kinetic Model for Methanol Conversion to Olefins, *Industrial Engineering Chemistry Process Design Development* 22, 532–538 (1983). DOI: 10.1021/i200022a031. (IF = 3.573).
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