

In memoriam

ZENO SIMON

23rd of April, 1935 – 21st of November, 2015

Zeno Gheorghe SIMON, Professor of Physical Chemistry at the West University of Timișoara, Romania, Corresponding Member of the Romanian Academy, died on the 21st of November, 2015, in Timișoara. He was a respected mentor, a good colleague, and a loving husband and father. His publications spanned various fields of physical chemistry and biophysics. His speeches, seasoned with a fine sense of humor, kept a sharp focus on the essence of the story. The audience will remember them and cherish the time spent with him.



MENTOR

To most of us, physical chemists and biophysicists, Professor Zeno SIMON was a mentor. Some of us were fortunate enough to work under his guidance, others had the opportunity to collaborate with him, and yet others were simply inspired by his ideas [4].

Professor SIMON published 344 papers, initiating important research avenues in quantum chemistry, computational chemistry, molecular biology, and cellular biophysics. He co-authored 14 specialty books: treatises, monographs, and lecture notes. He also wrote 2 popular science books, guiding his readers in fast-moving research fields, opening their appetite for interdisciplinary research, and carefully crafting the border between known and unknown [26].

Zeno SIMON earned his PhD in Physical Chemistry in 1965 from the University of Bucharest, under the guidance of Ilie G. Murgulescu, Professor of Physical Chemistry and Member of the Romanian Academy. During his PhD studies, working in Bucharest at the Research Center for Physical Chemistry of the Romanian Academy, he applied quantum chemistry (the Hückel molecular orbital method [5, 6, 38]) to investigate organic molecules (stability, *cis-trans*

isomerization, and electronic spectra). His works from this period appeared in prestigious journals from Romania, but also in leading journals from abroad [1, 16]. His collaboration with A.T. Balaban shed light on the electron spectra and stability of aromatic compounds [3]. Their studies were published in top journals [26] and highly cited books [2].

In 1965, Zeno SIMON returned to his home town, Timișoara, being appointed researcher at the Center for Chemistry at the Timișoara Branch of the Romanian Academy, and Associate Professor of Physical Chemistry at the University of Timișoara, Faculty of Physics. In 1971, aged 36, he became Professor and PhD coordinator. In Timișoara, he finalized his chemical kinetics studies on the molecular biology of the cell. Started in Bucharest in collaboration with Prof. Eli Ruckenstein, these works outlined a detailed modeling framework for understanding RNA synthesis, gene regulation, and protein synthesis in eukaryotic cells [24, 35, 36].

In the early 1970s, Timișoara hosted the birth of a powerful research group on quantitative structure-activity relationships (QSAR). This group was orchestrated by Professor Zeno SIMON for the next four decades. Their first paper appeared in 1972, opening the way to tens of seminal papers and two books published abroad [2, 28]. Their most cited works present an original approach to QSAR, the minimal steric difference (MSD) method, which was refined and became widely known as the minimum topological difference (MTD) method.

In most of his projects, Professor SIMON devised simple methods to tackle complex problems. He applied them to solve problems of interest in the scientific literature. Then, he gradually increased the complexity of his approach. He disseminated his results in the primary literature, as well as in state-of-the-art monographs of international visibility. In times when being visible abroad was an act of courage and required much effort, Zeno SIMON and his collaborators managed to push forward the frontiers of chemistry, being acknowledged by peers all over the globe.

In 1977, Professor SIMON moved to the Institute of Medicine of Timișoara, currently the “Victor Babeș” University of Medicine and Pharmacy Timișoara. In the two decades spent there as Head of the Biophysics Discipline, he focused on mathematical models of the cell cycle, as well as of gene regulation (for details, see the next section). Based on a kinetic model of the cell cycle, he predicted a linear relationship between the mean cell volume and cell cycle duration, a result observed experimentally in slowly growing bacteria [26]. In collaboration with Gheorghe I. Mihalaș, applying numerical methods to solve systems of differential equations, he investigated the role of positive control in gene activity regulation [10]. Their kinetic study of two interacting genes, p53 and mdm2, revealed an oscillatory behavior, with a possible role in cancer development [13].

Professor SIMON was elected a corresponding member of the Academy of Medical Sciences (ASM) in 1994, then full member of ASM and corresponding member of the Romanian Academy in 1997. In subsequent years, he coordinated a research group at the Institute of Chemistry of the Romanian Academy, Timișoara Branch.

FRIEND AND COLLEAGUE

Zeno's teamwork skills were as remarkable as his talent for exact sciences. He could seamlessly integrate into multidisciplinary research teams, build such teams, and maintain long-term professional relationships.

Edward Șeclăman, Associate Professor of Biochemistry at the "Victor Babeș" University of Medicine and Pharmacy, remembers him as follows: "I first met Professor SIMON during my MSc studies. From the very beginning, I was amazed by his brilliance in mathematical modeling of biological systems. After graduation, I was lucky to have had him as my PhD advisor. I will always remember what he taught me, his jokes, and his philosophy of life. Professor SIMON was an exceptionally creative, gifted scientist, and simply a good man!"

Alexandru T. Balaban, an organic chemist, member of the Romanian Academy, Professor Emeritus at Texas A&M University, Galveston, TX, USA, remained a lifelong friend and coworker of Zeno SIMON. He presents Zeno in a vivid narration: "My lifelong friendship with Zeno SIMON started in the 1960s, when he was the best qualified young quantum chemist from the school of Professor Ilie G. Murgulescu, and I was one of Professor Costin D. Nenițescu's collaborators. Our first joint paper was published in 1962, and by 1966 we had already published together, in Romanian and foreign scientific journals, nine communications using Zeno's computations. Our tenth joint paper was published in 1982.

Along with quantum chemistry, Zeno was interested in biochemical applications. He imagined an original method (minimal steric differences) for superimposing molecular structures without restrictions involving normal valences, in order to find correlations between chemical constitution and biological activities.

Together with Adrian Chiriac and one of my PhD students recommended by Zeno, Ioan Moțoc, we decided to publish a book: A.T. Balaban, A. Chiriac, I. Motoc and Z. SIMON, *Steric Fit in Quantitative Structure Activity Relations, Lecture Notes in Chemistry* No. 15, Springer Verlag, Berlin, 1980. A tragi-comic adventure illustrates the problems facing research and publications during those times. Since the book was to be photo-printed, the publishers sent us the special white paper, and we hired a professional typist and a specialist with templates for drawing chemical formulas. In order to be allowed to send the manuscript abroad, we had to obtain authorization; after waiting for a few weeks, the manuscript was

returned with each page adorned with the stamp APPROVED. Of course, we had to start again from the beginning – getting the special paper, and so on. We never photo-printed anything since then.

Later we published one more book together with two specialists in cancer research: N. Voiculescu, A. T. Balaban, I. Niculescu-Duvaz, Z. SIMON, *Modeling of Cancer Genesis and Prevention*, CRC Press, Boca Raton, Florida, 1990.

Zeno's scientific successes led to his election as a corresponding member of the Romanian Academy in 1997. Subsequently he became involved in coordinating research activities at the Timișoara Branch of the Romanian Academy. By then, I was Vice-President of the Romanian Academy, and we met several times yearly. After my mandatory retirement from the Bucharest Polytechnic University and my move as tenured Professor at the Texas A&M University in 2001, we still met when I traveled regularly during the summer to Romania. Also our families had become friends, and we were reading with pleasure and interest Stela Simon's memorial books."

A prolific period for his scientific work was the time when he worked as chair of the Department of Biophysics of the Timișoara Institute of Medicine, today "Victor Babeș" University of Medicine and Pharmacy. He continued his QSAR (Quantitative Structure – Activity Relationship) studies – various applications of MDM method (Moment Distribution Method) [29, 34] and developed his MTD method, based on minimum steric difference, published by Wiley [28, 33, 39].

Actually, he was also incited by the availability of a pretty good computer facility led by Gheorghe Mihalaș. Thus, a long-lasting collaboration started with him, having more than ten papers published together. All these theoretical studies started with the development of a mathematical model of a biological process, then translating the model into a computer simulation and discuss the behavior of the system. Several biological processes have been approached: drug-receptor interaction [11], gallstone formation [12] or the immune response [7, 14], starting from a model developed by Perelson [18]. But the preferred topic concerned regulatory processes of protein synthesis. Resuming some of Professor SIMON's previous work [20, 21, 23, 24, 35, 36], new versions of the models have been built, followed now by computer simulation studies. It was interesting to demonstrate how a system controlled by a positive feedback can reach stability [10, 30, 37]: actually, these systems have multiple steady states. These findings have led to the development of a more general mathematical framework of gene autoregulation [31, 32], including later also a quite common feature – the inter-related genes [15, 17]. The models became more complex: as the regulatory processes are threshold phenomena [8], the simulation programs had two running versions: one with stepwise change of parameters values and another one with a continuous function which imitates it closely. Moreover, the feedback loop is time consuming,

hence an appropriate frame for introducing a time delay in our models had to be developed [9]. Nevertheless, for such cases, the interpretation of the results turned out to be difficult, since in certain instances, small variations of input data (usually the initial relative concentrations and reaction rates) could yield tremendous changes in system behavior. That is why the applications have been tested on systems for which such data were available; more concretely for the synthesis of protein p53, which is controlled by MDM2. As the oncogene p53 was intensely studied, several data could be found in the literature. One of the most cited papers resulting from these studies referred to the oscillatory behavior of the p53-mdm2 system [13], as confirmed also by other studies [19].

He was also the founder and first dean of the Faculty of Pharmacy of the “Victor Babeş” University of Medicine and Pharmacy in Timișoara.

Besides his outstanding scientific results, we should mention here also his personality as a colleague and a true man of justice.

Often coming to work by bike, he never wanted to be remarked in elegant clothes or due to the tone of his voice. He was a very modest person, with a refined sense of humor.

HUSBAND AND FATHER

Zeno SIMON was born in Timișoara on the 23rd of April, 1935. His mother, Edith Simon (born Metz), had German origins: she was the daughter of Gisella Fronius from Vârșeț, Serbia, and Julius Metz, a Transylvanian Saxon (*Sächsisch*) from Sebeș Alba. His father, Virgil Simon, was Romanian, the son of Persida Simon (born Pârvu) from Caransebeș and Lazăr Simon, a lawyer from Ciacova. Virgil Simon himself graduated from law school and became a lawyer in 1922 [22]. Edith Metz studied decorative arts in Vienna. They married in 1932.

Living in an apartment on the Wilhelm Mühle Street in Timișoara, surrounded by his parents and grandparents, occasionally taken care of by a babysitter, Zeno's life had a comfortable start.

Then, in the summer of 1938, after a trip to Moneasa, he complained that “Mom, I feel like ants are swarming on my leg!”. Edith called her brother, the physician Alfred Metz. Listening to the symptoms, he exclaimed “*Mein Gott, das Kind hat Kinderlähmung!*” (“My God, the child has poliomyelitis!”) [25, p. 8]. This viral infection profoundly marked his life. As he puts it in the opening chapter of his memories, “According to the medical statistics of those times, I got over it quite easily. Just ‘sequelae’ at my left leg. I couldn't run anymore, I needed to use a walking stick (sometimes two), I couldn't fight with kids of my age, which often enraged me.” [25, p. 7]. For long distances he also wore a prosthetic shoe on his left leg. He had many toys, and he mostly played alone. Sometimes he played with

children from school and from the neighborhood. Nobody made fun of him because of his infirmity [25, p. 23].

Virgil Simon, a respected lawyer and member of the National Liberal Party, was not recruited during World War II. Nevertheless, times got rough, and, in 1940, he decided to buy a vacation house in Moneasa, where the family could spend some time away from the hectic life of the city.

In April 1944, fearing the British/American bombardments, the Simon family moved to Moneasa. Here they enjoyed the quiet life of the countryside, the beautiful landscape, friendly people, and delicious food. At 80 years of age, he still remembered the fried mushrooms he ate as a kid at a peasant family from Pietroasa [25, p. 37]. Nevertheless, news were flowing in about atrocities endured on the battle front by relatives of the people they met. The bombardments reached Timișoara soon. His father was there, but managed to reach shelter before their house was destroyed [25, p. 39].

Zeno continued his second grade at the elementary school from Moneasa. Here he met a teenage boy, a refugee from Bucharest, who had an amateur chemistry lab at home. Writing about this boy in his memories, Zeno relates that “I think he inoculated me with the passion for chemistry” [25, p. 37].

Later, by the age of 14, his interest for chemistry was fueled by the books and laboratory equipment offered as a gift by his uncle, Alfred Metz. Among these, he fondly mentions the book *Atoms* by Jean Perrin. His uncle taught him the most important safety rules to be followed in a chemistry lab. In his amateur laboratory, Zeno performed several experiments without any incident. He also presented some of them during chemistry class, in the 10th grade, at the “C.D. Loga” high school [25, p. 66].

On August 14th, 1952, Zeno SIMON traveled to Bucharest to take the exam for admission to the Biochemistry program of the Faculty of Chemistry at the University of Bucharest. He ranked first at the exam, being admitted with a fellowship that covered his living expenses.

Ironically, during the night spent by Zeno on the train, his father was arrested, along with other members of the National Liberal Party, deemed enemy of the state, and deported to the forced labor camp of Poarta Albă. Virgil Simon returned home in the spring of 1954. For years, Zeno was tried by a deep sense of guilt because he did not accept his father's offer to join him to Bucharest. He felt that his father might have escaped detention if he had not been at home during that night [22, p. 297].

In Bucharest Zeno SIMON was appreciated as an exceptionally talented student. No questions were asked about his middle-class origins, or his father's political detention. He got soon involved in research. After graduation, he became a PhD student under the supervision of Acad. I.G. Murgulescu.

Returned to Timișoara, in the summer of 1965, he met Stela Maria Leona Botiș in an encounter orchestrated by their parents. She was tiny and sweet, three years younger than Zeno, born on October 16th, 1938. Her mother, Adela Irina Stela Botiș (born Baciuc), was the daughter of Leona Baciuc (born Kormoș Alexandrescu) and the lawyer Aurel Baciuc from Târgu Mureș. Her father, Emil Botiș, was the son of reverend Teodor Botiș from Arad, and Maria Botiș-Ciobanu, originated from a family of miners from Roșia Montană. Educated in Romanian literature in Budapest, Maria Botiș-Ciobanu was a poet and writer. Her general culture and independent personality had a strong impact on Stela [22, p. 107]. Under the pressure of times Stela decided to study agronomy. Nevertheless, she chose to work as a librarian at the University of Agricultural Sciences and Veterinary Medicine from Timișoara, and later became a writer herself.

None of them believed in the success of this meeting, and both were wrong. It was love at first sight! They got engaged on August 14th, and married on September 2nd, 1965. Regarding their honeymoon, Stela writes that “we spent it in Bucharest bathed by honey-colored sunshine and in a short trip to the monasteries of Moldova”. She continues: “I utterly longed for becoming a mother, as soon as possible ...” [22, pp. 434–435].

Their son, Horațiu, was born on the 27th of June, 1966. They were proud and happy parents! Life in the Socialist Republic of Romania was “supportable” in those days. It gradually deteriorated during the next two decades, making it a challenge to procure the food for the family.

Horațiu went to the same high school as Zeno did, “C.D. Loga”, and subsequently studied physics at the West University of Timișoara. He was nurtured and encouraged by his parents to become an honest and performant person. Aged 20, he married a colleague, Gudrun. Graduating with highest honors, he pursued a PhD in theoretical physics at the University of Bonn. In 1993 Horațiu and Gudrun emigrated to Germany. At present, Gudrun is a high school physics teacher, whereas Horațiu is Senior Software Developer at SAP A.G., Germany. They have two children, Sieglind and Jan, and live in Heidelberg.

A loving wife and “the happiest mother in the world”, Stela Simon describes her marriage in these terms: “I had a *motto*: don't avoid any effort, keep going... Living with a man preoccupied with his work, day by day, for hours in a row, was anything but easy. Sometimes he was totally absent from the family's life (with all the affection he felt for us!). When I was young, I found all these things natural. [...] What stunned me, though, was his lack of knowledge of my intellectual preoccupations ...” [22, p. 436].

Professor Zeno SIMON knew the price of the peace of mind that enabled his scientific accomplishments. He acknowledged that his wife “managed and mainly carried out the household tasks. Her husband (the undersigned), animated by the ambition to accomplish something in the field of chemistry, placed the accent on his job and scientific work, being of little help at home.” [22, p. 518]. He expressed

his deep gratitude to his family in the closing sentence of his retrospective article [27]: “I am grateful to my parents, who, several decades ago, in difficult times, invested their last resources in my professional, but also general-cultural education; and to my family, my wife who had to accept an often absent minded father and husband.”

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G.I. MIHALAȘ, MONICA NEAGU, A. NEAGU[#]

“Victor Babeș” University of Medicine and Pharmacy, 2 Eftimie Murgu Square,
300041, Timișoara, Romania, [#]e-mail: neagu@umft.ro