

Citation for the nomination of Prof Rafiqul Gani for the EFCE's Jacques Villermaux Award

Prof Rafiqul Gani is one of the leading Chemical Engineers of his generation. He has been one of the leading researchers in Process Systems Engineering for several decades recognized throughout the world. He has been chair of the European Federation of Chemical Engineers Working Party on Computer Aided Process Engineering from 2006 to 2012, and Editor in chief for the main journal in the field, Computers and Chemical Engineering (CACE), from 2009-2015. He has also been a consultant to many companies and more recently set up his own consultancy, PSEforSpeed. He recently retired from the Technical University of Denmark where he has spent most of his career as researcher, teacher and mentor to many young researchers in Process Systems Engineering.

Professor Gani is an internationally eminent scholar well known for his contributions in four key research areas: **Computer aided modelling; Computer-aided molecular-mixture design, Computer-aided process engineering; Process tools integration.** Prof. Gani has published 208 papers in peer-reviewed international journals, over 157 papers in reviewed conference proceedings, 5 edited books, 27 book chapters, and over 300 presentations at various international conferences all over the world including 64 plenary/keynote lectures since 1995 and another 35 invited seminars. Total citations and h-index of Prof Gani are: 15419 and 61 in Google Scholar; 9667 and 50 in SCOPUS 3058; and 32 in ISI Web of Science (Jan 2019). His numerous invited lectures at international conferences and honorary academic lectureships, along with prizes and extensive citations in international journals, clearly attest to Prof. Gani's international stature and impact in the field.

Computer-aided Modelling: Models, in different forms, play a central role in almost all of PSE related activities. Prof. Gani has made outstanding contributions in three specific areas: development of generic process models; development of predictive models for properties of molecules-mixtures and development of computer-aided tools for modelling. Indeed, his very first papers were on generalized models for distillation columns (CACE, 1988) that are still regarded as one of the most detailed and complete. His latest papers have focused on development of generic models for crystallization operations (CACE, 2013). In the area of modelling of properties of molecules and mixtures, Prof. Gani's papers have pioneered the development and use of the group contribution concept. One of his papers is among the top 25 downloaded and cited papers of the *Fluid Phase Equilibria* journal (427 in ISI; 470 in SCOPUS and 631 in Google Scholar). The models from Prof. Gani's work are routinely employed in chemical process/product design and are also available in most commercial simulators (ASPEN, PROII). More recently, Prof. Gani's group developed a systematic modelling framework, and accompanying computer-aided modelling tools, that have been demonstrated to significantly reduce the time and human resources employed in the modelling process. His book (with Prof Ian Cameron) on "Product and Process Modelling: A Case Study Approach" (2011, Elsevier) is used as the text-book for many graduate level courses on computer-aided modelling around the world.

Computer-aided molecular-mixture design: The process of discovering or designing new materials and products possessing desired physical, chemical and biological properties is an important endeavor in the Chemical Process Industries and other related industries. Experimental data and statistical techniques alone cannot “discover” new materials; rather the key is to extract knowledge from the huge data sources using all applicable fundamental science and engineering so as to intelligently guide the search. To address this need, Prof Gani and his group have pioneered the development of a novel model-based technique for computer aided molecule and mixture design (CAMD). His first paper published in 1983 (in Fluid Phase Equilibria) is considered by many as laying the foundation of CAMD related activities within the PSE community. His paper published in 1991 (in AIChE journal) was included in the virtual issue on chemical product design, selected on the basis of the number of citations received (115 in ISI, 125 in SCOPUS and 162 in Google Scholar). His review paper on chemical product design published in 2004 (in CACE) continues to attract citations from almost all published papers on computer aided chemical product design.

Computer-aided process engineering: The development of model-based systematic methods and tools for chemical and biochemical process design has also been one of the main areas of research for Prof Gani. He has developed systematic methods for separation process synthesis and design with focus on distillation, membrane-assisted operations and crystallization. Also, since many of the separations need solvents, he has adopted his CAMD technique for separation process specific (extractive distillation, liquid-liquid extraction, crystallization, organic synthesis) solvent selection simultaneously with process design. This method is now routinely used in a wide range of industries (petrochemical, chemical, agrochemical, pharmaceutical, to name a few). Concerns for environment and sustainability have led Prof Gani to adapt and further extend his model-based process synthesis-design to systematic model-based methodology for design of more sustainable chemical and biochemical processes with special emphasis on process intensification. His recent papers on sustainable process design together with modelling and design of separation processes continue to attract citations and interest from academia and industry.

Furthermore, Prof Gani's research group developed a very successful software called ICAS (Integrated Computer Aided System) with tools for property prediction, computer-aided modelling, computer aided molecular-mixture-flowsheet design, process synthesis-design, solvent design, sustainability analysis, LCA analysis, cost analysis and many more. ICAS is not sold commercially but made available to the 30 member companies of the industrial consortium that supported his research group at DTU. Currently, more than 70 educational licenses have also been issued.

Service to Computer Aided Process Engineering: Prof Gani has established through Elsevier, the Computer Aided Chemical Engineering book series, which publishes the reviewed conference proceedings of ESCAPE-events as well as edited books on selected topics, such as Software Architecture, CAMD and Product Design. He served as editorial advisory board member and editor of *Computers & Chemical Engineering* before becoming editor-in-chief in 2009. He also serves in the

editorial advisory board of other journals (for example, Current Contents of Chemical Engineering) and regularly serves as guest editors for other journals including the October 2004 issue of the EFCE journal, Chemical Engineering Research and Design.

Service to the Profession of Chemical Engineering: Prof. Gani's leadership and service to our profession at the international level is simply outstanding. He has been very active in the EFCE, AIChE, and EURECHA (European Committee for the Use of Computers in Chemical Engineering Education) in various leadership capacities for over 25 years. He has chaired or co-chaired well over thirty-five international meetings, conferences, and sessions in the areas of computer aided process engineering, process systems engineering, computer aided molecular and product design, and computer aided modelling, as well as general Chemical Engineering (such as the 6th European Congress of Chemical Engineering in Copenhagen in 2007). He was instrumental in the foundation of the well-known ESCAPE (European Symposium of Computer Aided Process Engineering) events and ran the first one in Denmark in 1992. He also organized ESCAPE-25 in Copenhagen in 2015. He has organized special sessions at AIChE annual meetings and also topical conferences sponsored by AIChE, such as the PDS (Product Development Symposium) in 2008 in USA. He has been a member of the scientific committees for the international Foundations of Computer Aided Design conference series, the Process Systems Engineering conference series (also global event), special workshops on chemical product design, sustainable process design and many more. He served as an academic trustee of AIChE's CACHE for 2011-2013.

Within the EFCE he served as the Chair of the CAPE working party of the European Federation of Chemical Engineering (EFCE), for two terms during 2001-2007, and then in 2012 was elected as the scientific vice president and in 2014 was elected as the president of the EFCE. During his time as EFCE President he saw through the transition to becoming a charitable incorporated organisation, oversaw the audit of EFCE and its move towards a more sustainable financial future, and oversaw the development of the Barcelona Declaration at the 2015 World Chemical Engineering Conference in Barcelona. The declaration states the key role of Chemical Engineering in global grand challenges and the need for greater investment in research and education by governments and private sector organisations.

This outstanding record of achievements in process systems engineering, in methodology development and in industrial impact, as well as in leadership and service to our profession, clearly make Prof. Gani an eminently deserving recipient of the Jacques Villiermaux Award.

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