The Riemann International School of Mathematics (RISM) in cooperation with Università degli Studi dell'Insubria, Politecnico di Milano, ICAP Sira, Mettler Toledo, DEKRA (Italia) and Istituto Marcelline Tommaseo organizes the 1st Congress on:

Mathematical Methods in Chemical Engineering and Beyond (MMCEB 2018)

13 and 14 December 2018, Villa Toeplitz, Varese

MMCE 2018 will provide a forum on the use of recent mathematical methods and tools for solving a number of relevant engineering problems.
The congress will be a unique opportunity to share experience on mathematical models (ODEs or PDEs, numerical approaches) specifically developed for studying typical phenomena arising in Chemical Engineering and beyond. Talks delivered both by mathematicians and chemical engineers, who are leaders in the field, will cover a wide range of topics of interest. From one side, engineers will propose a variety of problems which are challenging to be worked out with standard or home made software. On the other side, mathematicians will provide useful tools for evaluating both the stability of innovative numerical methods for PDEs and ODEs and the reliability in the real world of the obtained solutions.

Detailed Program: December 13

09:15 - 9:45	Registration
09:45-10:00	Opening at the presence of the Deputy Rector Prof. S. Serra Capizzano and the Head of the Department of Science and High Technology Prof. U. Piarulli.
10:00-10:40	"Flow Chemistry Engineering: Innovations, Sustainability, and Real-World Opportunities with Outlook on Process Automation and Machine Learning"; **University of Adelaide**; V. Hessel
10:45-11:25	**Break**
11:30-12:10	"The GLT class as a Generalized Fourier Analysis and applications"; **Università degli Studi dell'Insubria**, S. Serra Capizzano http://www.rism.it/doc/abs-glt-model_2018.pdf
12:15-12:55	"APPLICATION OF NEURAL NETWORKS IN CHEMICAL ENGINEERING: new concept or old approach"; **Warsaw University of Technology**, E. Molga *The main applications of neural networks in chemical engineering are related to process control, data analysis and transformation as well as to process modelling.* *In this study a comprehensive survey of neural networks application in chemical engineering is given and characterized. Then, two fundamental approaches to neural modelling - a global and a hybrid one, respectively - are distinguished and described. Finally, a new aspect of neural modelling, which is related to application of ANNs for practical implementation of the third paradigm of chemical*

	engineering is considered.
13:00-14:25	**Lunch**
14:30-15:10	"A constrained model for MEMS with varying dielectric properties"*;* **Leibniz Universität Hannover,** C. Walker *An idealized electrostatically actuated microelectromechanical system (MEMS) involving an elastic plate made of a heterogeneous dielectric material is considered. Starting from the electrostatic and mechanical energies, the governing evolution equations for the electrostatic potential and the plate deflection are derived. A reduced model for the plate deflection is then obtained by letting the aspect ratio of the device tend to zero. The qualitative behavior of solutions to the resulting semilinear parabolic equation with constraint is analyzed.*
15:15-15:35	"From semi-batch to continuous processes: an analytical solution for copolymerisation"; **Politecnico di Milano**, F. Florit *In the framework of process intensification, a general kinetics-free transformation procedure of semi-batch processes into continuous ones was proposed, by adopting tubular reactors with side injections. A classical semi-batch process is copolymerisation, where the proper tuning of one monomer feed rate is crucial for quality reasons. For simplified kinetic schemes, an analytical solution to both feed rate policy and transformation problems was found. The resulting continuous process guarantees the same product quality of the discontinuous one.*
15:35-15:55	"Dust severity and safety issues as a function of the particles diameter"; **DEKRA Italia**, A. Fumagalli *In 2017, 164 accidents had involved powdered materials demonstrating that dust explosions are even today difficult to deal with. To protect against such phenomenon, the deflagration index is one of the most recognized parameters. The particle size distribution has a crucial role on it. Hence, a simple but reliable mathematical model has been proposed and validated to describe the effect of the mean particle diameter on the deflagration index, which is usable to identify dust severity and safety issues.*
16:00-16:40	**Break**
16:45-17:05	"An effective numerical approach for Dual Reflux Pressure Swing Adsorption detailed modelling"; **Politecnico di Milano**, E. Rossi *When modelling cyclic adsorption problems, the related conservation equations inevitably form a system of coupled non-linear partial differential equations. The attended solution is characterised by sharp gradients of concentration, both in space and time. To deal with this issue, a Finite Volume Method based numerical approach was developed and an efficient resolution strategy, combining different interpolation schemes and tailored for modelling specific features of Dual Reflux Pressure Swing Adsorption (DRPSA) processes, was set up. This way, an accurate detailed modelling of DRPSA, in reasonable computational time, is achievable.*
17:05-17:25	"Simulation of Runaway Phenomena in Controlled Plug Flow Reactors"; **Università degli Studi dell'Insubria**, M. Barozzi *In the last decades, tubular reactors (also known as Plug Flow Reactors, PFR), have found an extensive application in chemical industry, spacing from catalytic oxidations to the intensification of discontinuous processes. The main advantage offered by these reactors consists in a strong reduction of reaction volumes, which is possible by the fast kinetic promoted by the segregated flow within the reactor. This feature is also well known to be the cause for the complex control of the*

	PFRs thermal profile, due to the high exothermic heat generated. For this reason, several studies about the safety of tubular reactor-based processes have been carried out. Many works have been focused on providing methods and dissertations on the safety analysis of these reactors, with the ultimate goal of making processes based on PFR ever more intrinsically safe and optimized. This work set two purposes: firstly, simulating a catalytic oxidation process in a tubular jacketed reactor, where the thermal profile is regulated by a Proportional – Integral controller; secondly, carrying out a complete parametric sensitivity analysis. The proposed mathematical model is represented by a partial differential equations system (PDEs). With the application of the Method of Lines, the solution of the system is achieved by discretizing the spatial derivatives obtaining a system of ordinary differential equation (ODEs). In the results, we outlined the variation of the temperature and concentration profiles with respect to different control strategies. The parametric sensitivity analysis which was carried out showed the shifting of the runaway boundaries due to the application of a temperature controller.
17:25-17:40	**Conclusions**
19:30	**Social Trip & Dinner**

Detailed Program: December 14

09:15 - 9:55	"Generalized solutions for strongly singular problems", **Accademia dei Lincei – Univ. Pisa**; V. Benci
10:00-10:40	"Non-Parametric Kinetics (NPK) as an original way of thinking in process modelling"; **IQS**; R. Nomen & J. Sempere *Modelling and simulation of chemical processes usually requires deep research in mechanistic aspects of the behaviour of chemical reactions, in addition to other peripheral characteristics of the system. However, such fascinating task requires lots of experiments, being very expensive and time consuming. Chemical engineers, we require accurate predictions to project and control chemical plants, but the interest in reaction mechanisms or mass transfer control of some reactions or transformations is generally restricted to academic research. The NPK method was originally created to obtain kinetic information from Thermal Analysis and Calorimetry data. It opens the door to simulate chemical reactions and physical transformations – i.e. crystallisation – using simple interpolation techniques. This communication will expose the basis of NPK and some of its applications.*
10:45-11:25	**Break**
11:30-12:10	"Mathematical modelling of complex reacting systems", **Politecnico di Milano**; E. Ranzi *Detailed kinetic mechanisms of pyrolysis and combustion of complex liquid mixtures, such as commercial fuels and refinery streams, are nowadays widely used not only at the research scale but also for industrial applications. This research area has significantly improved during the last years thanks to new experimental techniques and mainly to powerful computational tools. This presentation will analyze the different facets of pyrolysis and combustion processes with particular attention to complex gas-phase kinetic mechanisms, moving from the very theoretical 'ab initio' studies up to the generation of large kinetic mechanisms. The attention will first focus on the chemistry and the kinetic models at the very theoretical level. Then, numerical and statistical methods, together with practical applications of kinetic mechanisms at the industrial scale will be briefly discussed.*

12:15-12:55	"Positive solutions of weakly coupled systems with critical growth in dimension two", **Chonqqing Jiaotong University**, J. Zhang *In this talk, we are concerned with positive vector solutions of Bose-Einstein type systems in dimension two. The interaction is of critical exponential type in the sense of J. Moser. We prove, using variational methods, the existence of positive vector ground state solutions both in the attractive and repulsive cases. This talk is based on joint work with Daniele Cassani and Hugo Tavares.*
13:00-14:25	**Lunch**