tusail

H2020-MSCA-ITN-2020

PROJECT #955661

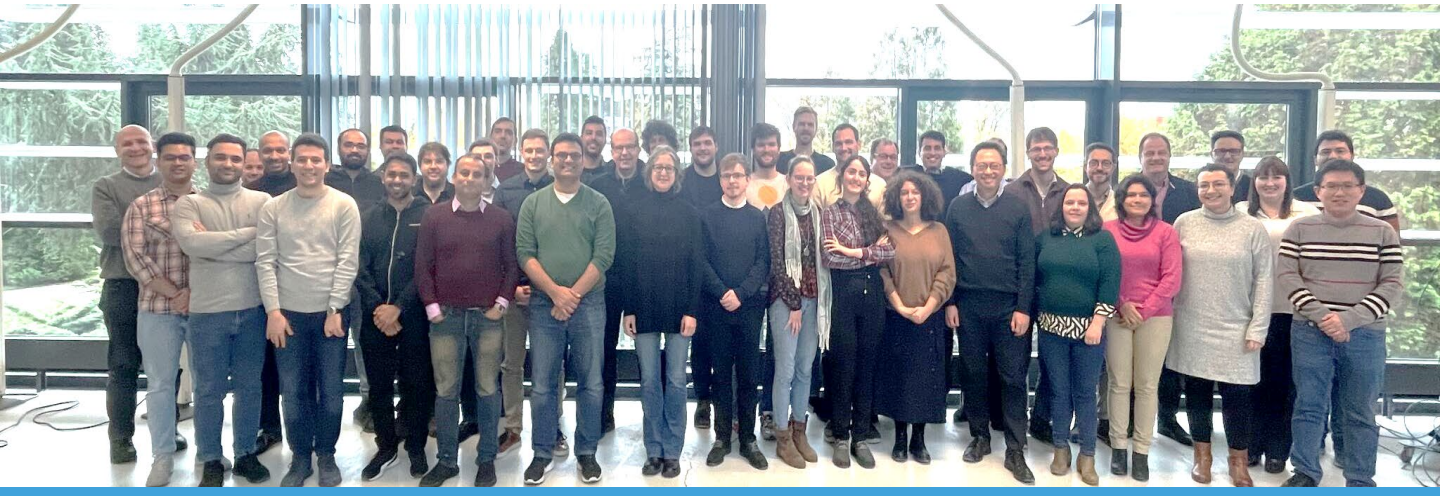
Planning outreach & public engagement

TUSAIL suffered a massive blow in January 2023 when Assem Zharbossyn (right), was killed in a Road Traffic Accident. She died instantly when she was hit by a car on her way home from work. This shocked and devastated all who worked with her. She was an ESR and an integral part of our collaborative research teams, working closely with colleagues from the University of Salerno and the University of Twente as well as the wider TUSAIL network. Assem began her project at the University of Salerno in 2021 having completed her Masters degree in Chemical and Material Engineering at the Nabarzayev University, Kazakhstan. She was engaged in experimental work to determine a protocol to calibrate parameters for DEM models using both primary and (coarser) meso-particles, focusing on mono- and bi-component powders. She was a highly motivated researcher who was seriously committed to her work. She was always supportive to her colleagues and ever eager to learn from others. A very promising researcher with great potential, she will be much missed by all who knew her.

In this newsletter, our ESR spotlight features four ESR profiles and we focus on TUSAIL's third Doctoral School, hosted by Universiteit Twente, Netherlands. Our scientific training programme continues apace, incorporating the design of outreach materials and exploring how we can effectively communicate our research to a broad spectrum of audiences. There was also an opportunity to catch up with ESRs from previous ITNs – TMAPPP and PARDEM – explore their experiences and find out about life after the ITN.

We recently held our 4th Doctoral School, hosted by DCS Computing GmbH, Linz… more on that in the next instalment.

Professor Jin Ooi, TUSAIL Project Coordinator



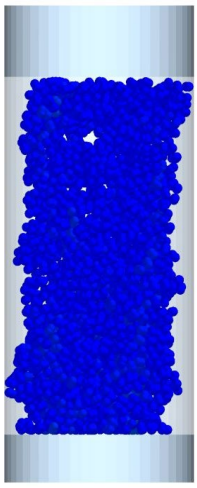
ESR Spolight

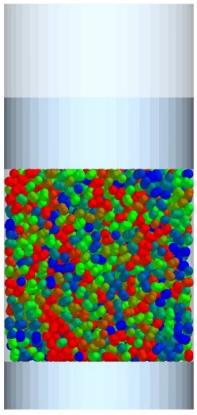
Interested in compaction of powdered material?

Our ESR Amine Ait Ouazzou is a passionate engineer in energy and propulsion systems, graduated from a Franco-German double degree program between the University of Kaiserslautern and INSA Rouen Normandie.

Within TUSAIL, Amine is working on multiscale models for reconstitution of compacted powders at the Institute of Process Engineering and Particle Technology, Hamburg University of Technology in partnership with Société des Produits Nestlé S.A. His aim is to develop advanced meso-particle models, which will be used to inform a macroscopic multi-dimensional PBM modelling considering main particle properties. Amine is currently focusing on tablet compaction at Technical University of Braunschweig for his secondment.

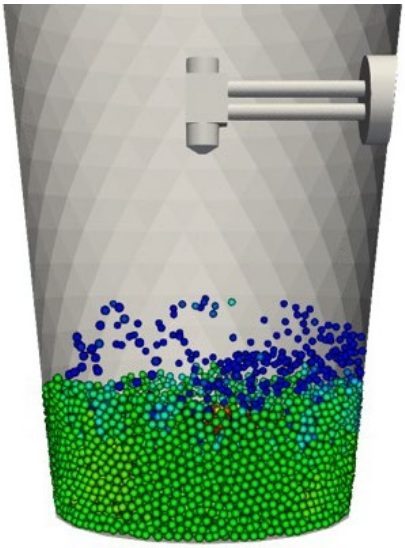
Amine is our language talent! Due to the travels he had during his studies, he speaks French, Arabic, English, German and learning Italian!





Are you interested in fluidised bed agglomeration?

Our ESR Gero Stöckl is a chemical and process engineer from Graz University of Technology, where he investigated the use of deep neural networks for heat radiation modelling in polydisperse particle systems.



Within TUSAIL, Gero is developing a dynamic flow sheet simulation that can predict agglomeration in fluidized beds across different scales. This will be achieved by informing a large scale PBM model using the results obtained from calibrated CFD-DEM simulations.
Gero is currently working on coupling CFD-DEM to PBM during his secondment at BASF SE in Ludwigshafen. This allows him to simulate pilot and industrial sized plants at low computational costs.

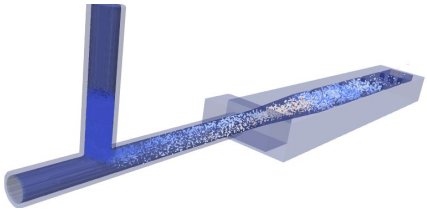
Gero is also hosted at Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, and will move to Siemens Process Systems Enterprise (PSE) in September 2023.

ESR Spotlight

What happens inside jet mills?

Our ESR Jobin Raju graduated as an applied mathematician from a joint degree program between Technical University of Vienna and University of L'Aquila, where he specialized in numerics and CFD for multi-phase flows.

Within TUSAIL, Jobin is developing a methodology to quantify particle breakage in jet mills using CFD-DEM and PBM. Different types of jet mills are subjected to experimentation to calibrate material breakage and fitting parameters to build a breakage kernel for PBM. CFD-DEM coupled simulations are used to extract data such as impact energy, collision frequency etc, from the lab scale mills under consideration. This information will be used to build the machine and material functions which in turn is used to inform a PBM. One of the key aspects of his research is to develop reliable upscaling methods for milling processes for industrial applications, specifically in the pharmaceutical sector.
Jobin is currently hosted at Institute for Particle Technology, Technical University of Braunschweig, and will move to DCS Computing, Linz, in October 2023.



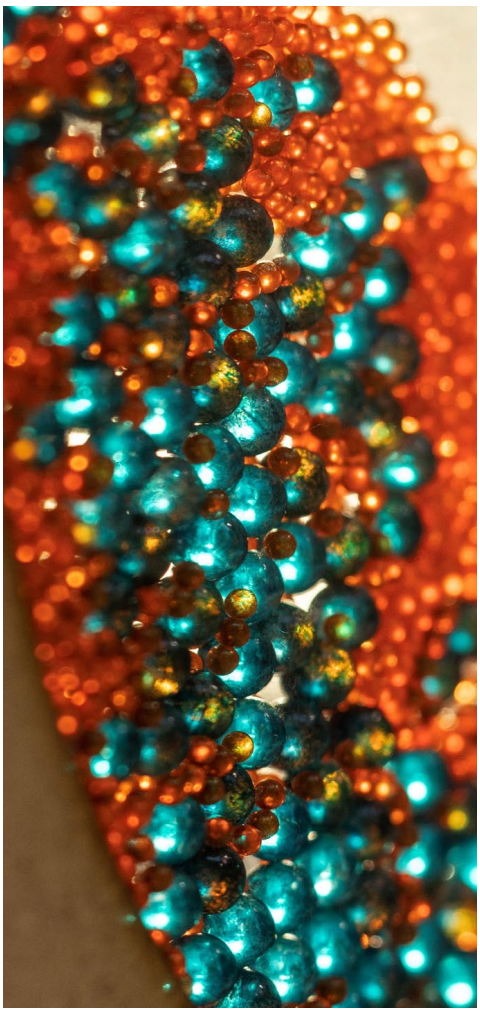
Are you interested in wet particle systems?

Our ESR Roxana Saghafian Larijani is a chemical and process engineer and graduated from the University of Tehran, where she focused on the CFD-DEM simulation of fluidized bed with non-spherical particles in the presence of an external electric field.

Continuing her research journey with granular systems, within TUSAIL she is investigating wet particle systems, particularly wet granulation process, in which the liquid bridge force among particles will lead to the production of enlarged particles or agglomerates. As a chemical engineer, it has always been her passion to find out what can increase the efficiency of the processes and the quality of the product. In this project, she is using DEM along with an upscaling approach (coarse-graining), which will reduce the computational cost of the simulations, to investigate the performance of industrial-scale granulators in different operational conditions.
Roxana is hosted at the University of Twente during her PhD and is currently undertaking her secondment in Johnson Matthey (UK), where she is conducting experiments for the calibration and validation of the CG-DEM model for wet systems.

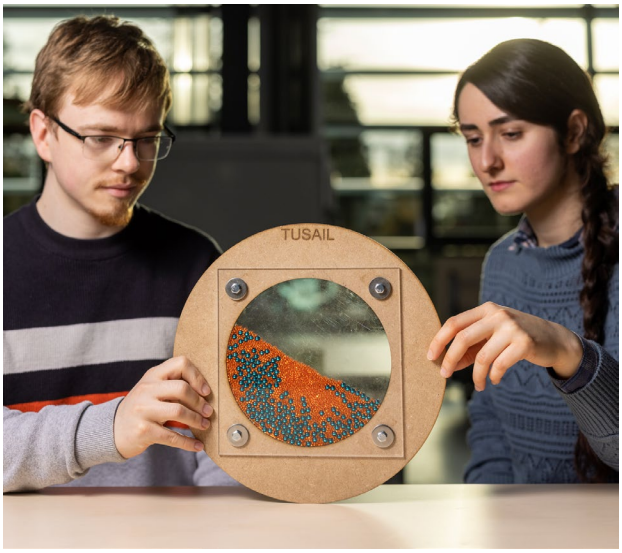
3rd Doctoral School

DesignLAB, University of Twente



At the beginning of our third Doctoral School, we spent two days at DesignLab UT to prepare, plan, design, and make useful, usable outreach materials. The DesignLAB has spaces specifically designed to inspire innovative thinking, promote collaborative projects, and support quick prototyping. Their workshop facilities include laser cutters, 3D printers, and other rapid prototyping tools, as well as multi-purpose rooms ideally suited for team projects. ESRs were joined by two guest postdocs, Floriana Anselmucci and Marta Stasiak, forming three groups to desig three demonstration models: a flow segregation, a fluidized bed and a rotating drum. These demonstration pieces were subsequently used by Retief Lubbe at the 2023's Girls' Day Event, hosted by University of Twente and organized by high school students and other ITNs. Going forwards, they will be shared across the consortium for other outreach activities involving the general public, especially focusing on budding young scientists.

In the pictures: Balázs Füvesi and Roxana Saghafian Larijani with the rotating drum (left), and Afshin Taghizadeh, Behrad Esgandari, and Akhil Mathews with the flow segregation demonstration instruments (right).



3rd Doctoral School

DEM Calibration and MercuryDPM Workshops

Two important training workshops were delivered by University of Twente and MercuryDPM. The first workshop focused on DEM calibration and specifically introduced a calibration toolbox called "Grain Learning". This tool uses machine learning techniques to estimate parameters in the Discrete Element Method. The workshop provided ESRs with hands-on experience using Grain Learning, and they had the opportunity to learn about its capabilities and limitations. The second workshop focused on the discrete-to-continuum transition, which is a critical concept in granular mechanics. MercuryDPM was used to analyse various granular systems and observe their behaviour at different scales.

ESR feedback: *these workshops were invaluable experiences for PhD students. They provided an opportunity to learn from experts in the field, gain hands-on experience with important tools and software, and expand their knowledge and understanding of granular mechanics.*

3rd Doctoral School

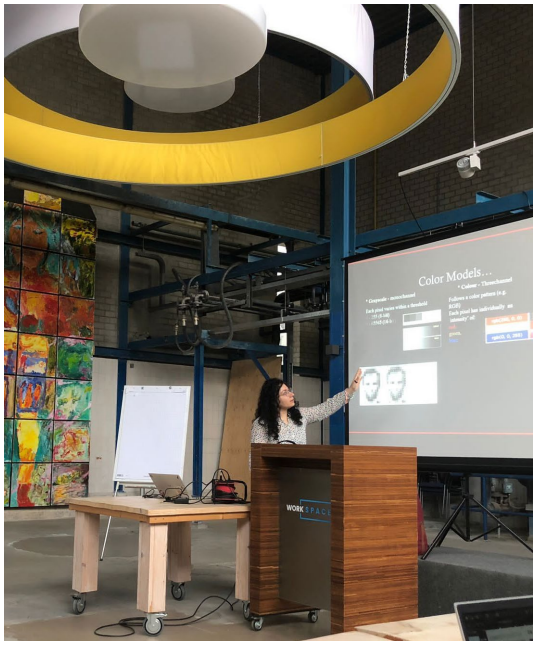
TUSAIL Science Program

Themed discussion rounds were the highlight of the third doctoral school at Twente. To exhibit their projects, ideas and progress, each ESR had a brief presentation on the topics that they have been working on. Each presentation was followed by feedback from the supervisors and the external advisors as well as a short discussion to identify potential collaborations. The external advisors - Prof. Christine M. Hrenya, University of Colorado, Prof. Alberto Di Renzo, University of Calabria, Dr. Luis Martin de Juan, Astra Zeneca, Dr. Luisa Orozco, eScience Center - were always available at the disposal of the ESRs. Their expertise in specific areas such as coarse-graining, breakage, agglomeration, PBM etc were very helpful in bringing forth new ideas during the themed discussion rounds. The discussions in this session led to broad insights into other ESRs' projects and also many interesting collaborations were identified.

The discussions were further continued in breakout groups with each of the ESRs displaying their project poster. The supervisors and the external advisors each joined the discussions and gave their valuable input on the respective themes. This session was later concluded by summarizing the discussion points from each of the ESRs and documented by Prof. Stefan Luding.

3rd Doctoral School

Courses on Advanced Computing and Analysis



A course on High Performance Computing (HPC) was conducted by Adam Belloum from the National eScience Centre. The lecture was dense in terms of content and introduced the concept of parallel processing for engineering problems. Parallel processing packages such as OpenMP and MPI were introduced to the audience with splendid working examples. This was followed by a session on image analysis by Dr. Floriana Anselmucci (photo on the left) who is a postdoc at the University of Twente. The session involved hands-on experience with image processing packages using Python. She explained ways to extracts meaningful data from granular experiments and exploiting it for particle tracking and DEM calibration.

The sessions were very helpful for those ESRs who are currently working on code development and post processing data.

Insight from ESRs from previous ITNs

ESRs enjoyed a delightful experience meeting alumni from previous ITNs – T-MAPPP and PARDEM. Each of the alumni members gave a short introduction about their whereabouts and their work domain. They shared their experiences during their doctoral research, and stories about how they made the best out of conferences and secondments. We had discussions about setting long term goals and how TUSAIL can be used to achieve them. The day ended with a social dinner at Twente Foedhal.

Highlighted Publications

Influence of Process Parameters and Particle Size Distribution on Mechanical Properties of Tablets

Amine Ait Ouazzou and colleagues studied the influence of the particle size distribution of maltodextrin powders with a dextrose equivalent level of 29 as well as two tableting process variables, namely the compression pressure and the dwell time, on the tensile strength, porosity, and pore size distribution of the final tablet. This study offers a better understanding of how the properties of a tablet are influenced by the inter-correlation of powder characteristics and tableting parameters. https://dx.doi.org/10.1002/cite.202200157

A comprehensive comparison of Two-Fluid Model, Discrete Element Method and experiments for the simulation of single- and multiple-spout fluidized beds

Behrad Esgandari and colleagues explore a comparison between TFM, CFD-DEM, and experiments; a new modification to μ(I)-rheology to consider rolling friction in TFM; examining the effect of two different frictional solids stresses in TFM; testing four different drag models in TFM and CFD-DEM; and using proper TFM closures to improve comparisons with CFD-DEM and experiments. https://dx.doi.org/10.1016/j.ces.2022.118357

Upcoming Conference

International Congress on Particle Technology (PARTEC)

The TUSAIL network will have its 5th doctoral school in Germany, hosted by the Technical University of Braunschweig. The first half of the doctoral school will partially run in parallel with PARTEC, where all TUSAIL members take part and scientific presentations of the ESRs are scheduled. This will accordingly take place in Nuremberg/Erlangen. The second part will take place in Braunschweig and will further educate the ESRs.

PARTEC is a global event that focuses on research and development in particle technology, and it is open to scientists and engineers from all over the world. The conference is held in English and covers a variety of topics related to particle technology, such as particle formation, agglomeration and coating processes, as well as industrial applications for particles. The conference will be held in Nuremberg, Germany between 26-28 September 2023. For further information, please visit https://www.partec.info.

PARTEC 2023
International Congress on Particle Technology

The Consortium

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