MATHEGRAM Newsletter

Issue No. 6 June 2023

We are pleased to welcome you to read the very last issue of MATHEGRAM Newsletter, as MATHEGRAM project is drawing to an end. We are also very pleased with the fact that the project as a whole went very well. Most ESRs have successfully completed their projects and move on to a new venture. We wish them every success in their career.

This issue of Newsletter includes not only Rafeal's secondment experience at the University of Surrey but also Sina's research report on his work at UNISA. In addition, a brief report on the MATHEGRAM symposium at the 4th Aspherix and CFDEM conference from Marina. I hope you enjoy reading the articles in this Newsletter.

I would like to express sincere gratitude to DCS Computing GmbH for organising our 2nd MATHEGRAM symposium in conjunction with the 4th Aspherix and CFDEM conference in Linz, Austria. We are so glad to be able to meet in person and showcase our research outcomes to a wider audience. It was a well organised and attended conferences, we enjoyed very much! We are also very proud of all MATHEGRAM ESRs for your hard work and collaborative attitudes, and for the amazing achievements you made! We wish you all the best of your next endeavor! To all MATHEGRAM partners, this may be the last time we meet as part of the MATHEGRAM project, but we have build something truly special for further collaboration. Let us keep exploring and keep in touch!

Once again I wish you all a restful, relaxing and productive summer and look forward to meeting and collaborating with you in future.

Prof. Charley Wu
MATHEGRAM coordinator

Inside this issue

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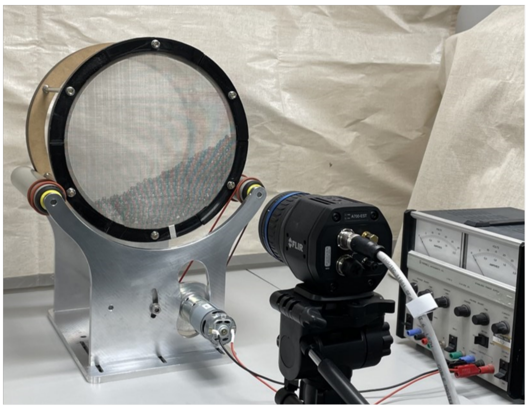
My secondment at the University of Surrey

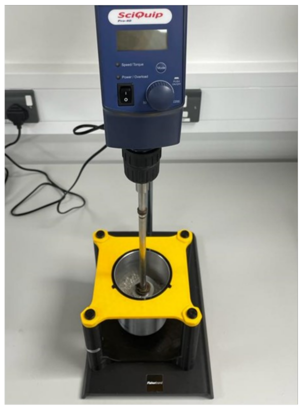
Rafael Rangel (ESR13, CIMNE)

After difficult times for face-to-face collaborations, I had the great opportunity to carry out my first secondment at the University of Surrey in Guildford, UK. This visiting period lasted four months, from February to June 2022. During that time, I had the pleasure to work with Professor Charley Wu and the members of his research team from the Department of Chemical and Process Engineering. Luckily, fellow ESR Francisco Kisuka, from the same department, was also carrying out a secondment at the same time. His research topic involves heat generation by energy dissipation during particle collisions. His plan was to perform experimental analyses on the subject, and so we joined forces together. The experiments were conducted in the Powder Technology Laboratory, where we had great assistance from the lab technicians. We also had the collaboration of other scientists from MATHEGRAM through fruitful discussions about the methodology and results, including Colin Hare from Newcastle University and Vincenzino Vivacqua from Johnson Matthey.

Francisco and I worked together on two experiments. Both of them aiming to measure the temperature rise during particulate flows in which particles are constantly colliding and sliding against each other. In one of the experiments, a rotating drum was used to agitate the particles, whose temperature was monitored with a thermal camera. Before starting this experiment, we were fortunate to have a lecture on infrared thermography during one of the training schools organised by MATHEGRAM, from which we gained valuable knowledge to prepare the setup. The other experiment consisted of a thermally-insulated beaker filled with particles that were agitated with an overhead stirrer. The temperature, in this case, was measured with thermocouples, which revealed surprising temperature increases of up to 50^{o}C, which even melt one 3D-printed impeller! In both experiments, different particle materials and operating conditions (e.g. fill ratio, rotation speed, etc.) were considered to investigate their effects on the generation of heat. We wrote two articles with the results obtained, one has been published in Powder Technology.

For me, working on laboratory experiments was a unique and exciting experience, as my research is mostly computational. This opportunity expanded my research horizons and I learnt a lot from my colleagues in Surrey. Now, I am back to the computer simulation world, where I plan to reproduce the same experiments. I will be doing so with other MATHEGRAM colleagues from the Imperial College London, where I am currently doing my second secondment and I could not be more excited.





Flow behaviour of zeolite powders at high process temperatures

Sina Zinatlou Ajabshir (ESR9, UNISA)

The thermally-induced deformation of a granular medium is an interesting phenomenon that can result either in an enlargement of voids or in their reduction whenever the medium is subjected to changes in temperature. As individual particles dilate with increasing temperature, internal instabilities at contact points may occur, which can then result in particle rearrangement – even leading to pore space contracting despite the increase in temperature. The overall mechanism can be difficult to assimilate at first and even tricky to quantify, so let's break it down into more palatable pieces.

Zeolite powders are an active ingredient for various catalytic processes, adsorbents and can also be used directly for selective laser sintering. During the zeolites manufacturing process, solid processing can become a hurdle due to the impact of processing conditions on powder flow. This, overall, would not only impact the manufacturing efficiency but also the quality of the zeolite. One of the important process conditions that changes during the manufacturing process is temperature. Temperature can change the particle properties affecting the powder flow properties and, therefore, the latter need to be tested at the process conditions.

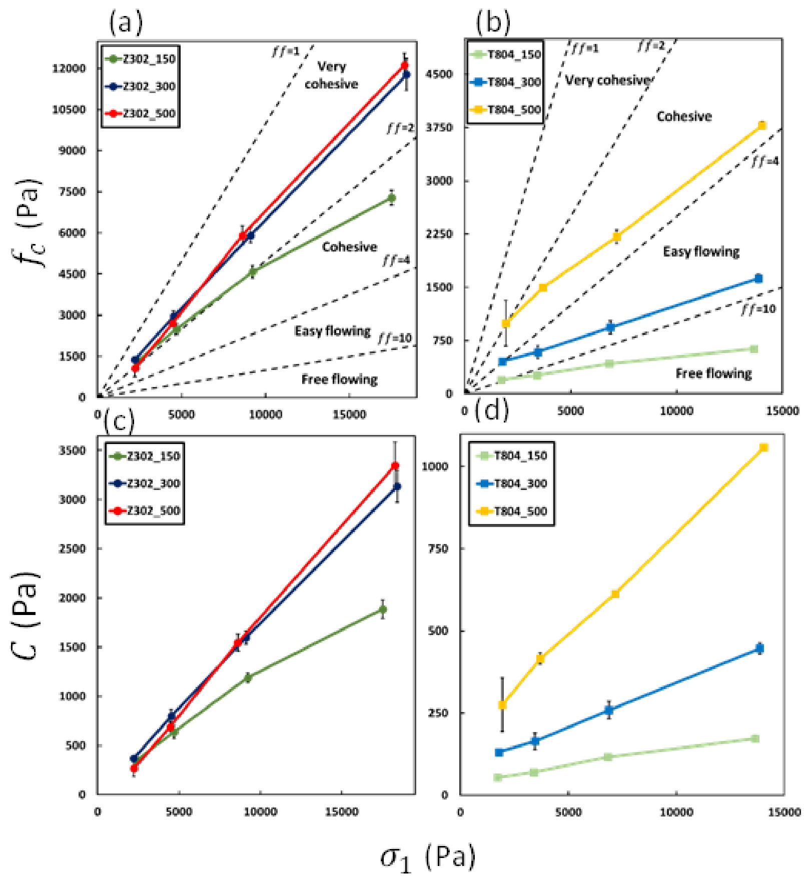


Fig 1: Flow functions: (a)Z302; (b)T804 and cohesion: (c) Z302; (d)T804 tested powders measured with an Anton Paar shear cell

The flow properties of two types of zeolite powders, Z302 and T804, were evaluated at temperatures of 150, 300, and 500°C in the range of 1-8 kPa of normal consolidation stresses by an Anton Paar shear cell. The two materials show a very different flowability behaviour, even at the lowest temperature tested. In fact, using the Jenike classification of powder flowability based on flow factors, at 150°C, the T804 zeolite is within the free-flowing range, on the other hand, the Z302 zeolite falls between the very cohesive and cohesive ranges. However, the temperature appears much more significant effect on the T804 zeolite at 500°C and the flow function falls into the cohesive range while the Z302 zeolite flow function changes only for large values of consolidation stresses, by showing a flow function falling entirely within the very cohesive range (Figure 1).

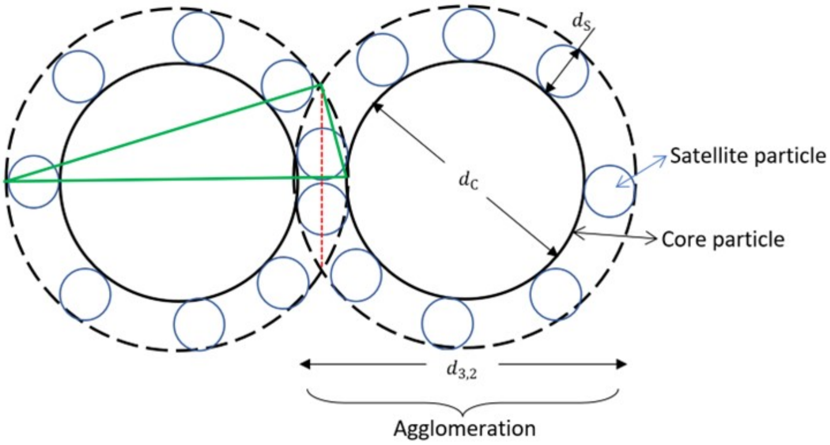


Fig 2: Model for agglomeration formation in zeolite powders

To find an explanation for understating such different behaviours of these two materials at changing temperatures and consolidation stresses, a theoretical framework was developed to take into account the different particle size distributions of the two powders (Figure 2). It was assumed, based on SEM images, that the particles in the powders are organized in agglomerates made of a single core particle and a number of minor satellite particles, therefore allow several multiple contact points between neighbouring agglomerates.

In fact, the large number of fines in the case considered on the one hand is responsible of the much worse flowability but, on the other hand, it determines two order of magnitude lower force intensities at contacts. This may also explain the less effect of material plasticization at the contact during consolidation, that is responsible for temperature dependence of the cohesion of materials mainly affected by van der Waals forces. So, in general, it can be confirmed that an adequate estimate of the average material fabric provides averaged estimates of contact forces that are able to explain the different behaviour of temperature and consolidation changes shown in powders.

A characteristic structural length was calculated for the two materials at all temperatures and major consolidation stresses to include the effect of the changing density on the powder flowability. In these terms, the results indicate an even worse behaviour to flowability of the more cohesive powder Z302 than detectable by looking at flow factors classification of the flow functions.

The Second MATHEGRAM Symposium

Marina Bortolotto (ESR 7, IC)

On the 21st of April, 2023, DCS Computing hosted a MATHEGRAM Symposium as part of the 4th Aspherix® & CFDEM® Conference in beautiful Linz, Austria. This was our final opportunity to meet in person and fortunately, most of the academic institutions were represented.

The work of 12 ESRs developed at 8 different institutions was successfully presented to a wider audience that included conference participants and MATHEGRAM members. The presentations all together definitely provided an overview of the entire project and highlighted its main achievements.

The symposium was a success, and it was a great opportunity to see the complete breadth of topics covered by MATHEGRAM, and all the great findings and achievements that our colleagues managed to accomplish, despite many unforeseen challenges we faced during pandemic. I am pleased to see that many ESRs now obtained their PhD degrees and are now officially a doctor in philosophy, and others (including myself) are doctors-soon-to-be. Great job, congratulations!

It was a pleasure to share this period with such brilliant colleagues that came from different parts of the world. Beyond the technical and academic experience, this project exposed me to different realities and cultural backgrounds that were so enriching. I hope our paths cross again in the near future! As we would say in Scouts in Brazil (free translation from Portuguese): “it is no more than a see you later […] soon enough we will see each other again.”

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