

Welcome to the 2nd issue of the IPROCOT newsletters! We hope you had a most enjoyable summer! We welcomed Mr Alon Mazar to become an early stage researcher to IPROCOT consortium.

Our 2nd advanced training course (i.e. ATC2) on “Multi-scale modeling of particulate product manufacturing: theory application” was a great success. We all had a wonderful and rewarding time in Albi, France In July! I’d like to express my appreciation to Ecole des Mines d’Albi for organizing such a successful event, and to all invited speakers and IPROCOT supervisors and international advisory board members for their contributions. You can find more information on IPROCOT ATC2 in this newsletter.



15 IPROCOT fellows at Ecole Des Mines d’Albi, France

We also had a very fruitful project meeting in July, where all IPROCOT fellows presented their progress on IPROCOT projects, which are very impressive. I am also very delighted to know that many of our fellows have started or already finished their first secondments, which to my opinion is a very good mechanism to train next generation researchers and to consolidate our collaborations. I hope our fellows enjoy your secondments and take full advantage of the opportunity to interact and collaborate with your host.

As reported in this newsletter, many IPROCOT fellows also started to present their research at national and international conferences, which are good channels to disseminate IPROCOT research and to network with researchers working in the similar areas. In addition, IPROCOT fellows have actively engaged in outreach activities ranging from contributing articles to the newsletter to participating science festivals (see page 6). Well done and keep it up!



IPROCOT supervisors at Albi, France

Finally, our mid-term review meeting and ATC3 are fast approaching. I look forward to meeting you all in Krakow, Poland soon.

Prof. Charley Wu
IPROCOT coordinator

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Granular Segregation in Tapered Rotating Drums

Sebastian González

Introduction

Segregation of granular materials can be found everywhere, but we are still far away from its complete understanding. If you shake your muesli the large nuts will go to the surface. And the same phenomenon is at work in pharmaceutical powders as well as in volcanic avalanches. By studying the evolution of a simple system, we can obtain data in the yet cleanest way, and use that data to find the free parameters of a continuum theory of segregation.

Results

Our setup is extremely simple: a bi-disperse mixture of particles is put in a rotating drum whose diameter increases along the axis of rotation. The geometry of the drum creates a fixed velocity profile that in turns generates segregation of particles according to size along the axis of the drum.

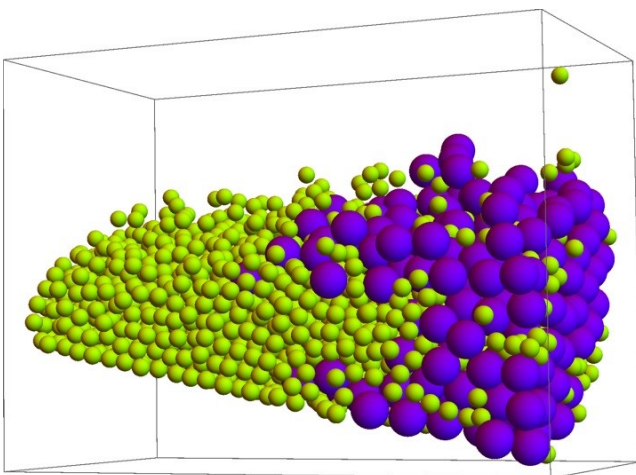


Figure 1 Snapshot of the system in the segregated state for a vertical cut along the rotation axis. Particles coloured by size

By looking at the evolution of the small particles' concentration along the axial direction as a function of time, the free-parameters of the Gray & Chugunov (2006) theory can be obtained, see Fig.2.

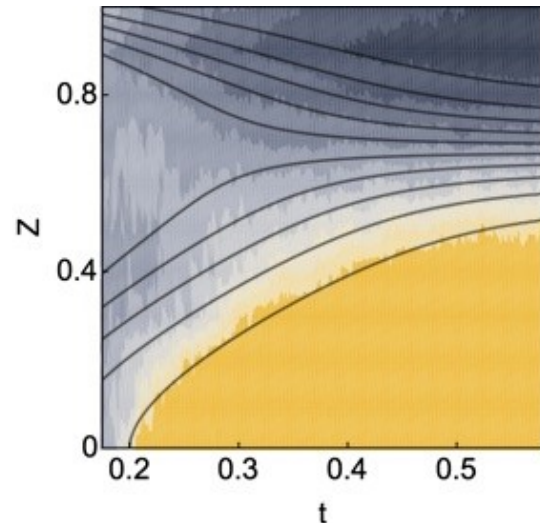


Figure 2: Concentration of small particles along the axial direction as a function of time. Colours represent the simulations' data while the solid lines are the fit from the theory

Conclusions

The system described could become a standard experiment to obtain the segregation parameters for a given mixture. With those parameters, the application of the continuum theory of Gray & Chugunov can be used directly in a wide range of configurations. In particular, this could be used to study the effect of segregation in roll compactors, for which computational modelling using the discrete particle method is not possible due to the large number of particles involved.

References

J. M. N. T. Gray and V. A. Chugunov, 2006, Particle-size segregation and diffusive remixing in shallow granular avalanches, *Journal of Fluid Mechanics* 569, 365-398.

The Second IPROCOM Advance Training Course

The Second IPROCOM advanced training course (ATC 2) on “Multi-scale Modelling of Particulate Product Manufacturing: theory and application” was successfully held in Ecole des Mines d’Albi, France, on 8th - 11th July 2014. This course brought together 45 participants from 18 nations. Lectures on a wide range of topics related to modeling and simulations were given by 11 international experts from France, UK, Austria, USA and China. IPROCOM ATC2 was reported in three different local media.



The ATC2 was well received and some encouraging comments from the participants include:

"The project meeting was well organized. During the first two days every fellow had the opportunity to present their own research and progresses, with a general discussion for each work package. It was very interesting to get new ideas and to better understand the different aspects of the IPROCOM project. For the ATC2, several topics were covered and explained by international experts. Therefore each fellow could learn useful knowledge that will be useful to their own research."

"ATC2 was very well organized and some of the lectures were really helpful for my learning and understanding of DEM and FEM."

"Coming from the field of continuum and multi-scale mechanics, I found the content of the lectures very interesting."

"The social activities were excellent, we had plenty of time to get to know each other and enjoy the fine food and sites of Albi."

"The lectures were well structured and were well related to my research interest."

IPROCOT members attended “Particulate Processes in the Pharmaceutical Industry IV” (PPPI-IV)

On 14-18th September 2014, IPROCOT members attended the international conference “Particulate Processes in the Pharmaceutical Industry IV” held in Postdam, Germany. They gave several presentations related to IPROCOT projects including:

“Compaction behaviour of dry granulated binary mixtures” given by IPROCOT fellow, Miss Lucia Perez Gandarillas.

“Characterization of bulk density distribution of roll-compacted ribbons using terahertz spectroscopy”, delivered by IPROCOT coordinator, Prof. Chuan-Yu Wu, who reported a collaborative work between the University of Surrey and Advantest. IPROCOT fellow, Miss Serena Schiano, is one of the main con-

tributors to this work that demonstrated the feasibility of terahertz imaging techniques in characterizing properties of powder compacts;

“Understanding of compaction processes using finite element methods”, a keynote lecture given by IPROCOT supervisor Dr. Abder Michrafy.

“Heuristic modeling of fine particle fraction and optimization of formulation for pulmonary drug delivery” by IPROCOT supervisor, Dr. Aleksander Mendyk.

IPROCOT members also had some in-depth scientific discussions with other delegates working in the similar areas and enjoyed the excellent networking opportunities at the conference.



Members of IPROCOT attended APS PharmSci 2014 conference



IPROCOT fellow, Dr. Andreja Mirtic (ER 3) and her supervisor, Dr. Gavin Reynolds, attended APS PharmSci 2014 conference at University of Hertfordshire in Hatfield, United Kingdom, on 8th - 10th September 2014. Andreja presented her work on “Influence of mechanical properties of pharmaceutical materials on milling of roller compacted ribbons” and Gavin Reynolds gave a lecture on “Proposal for a Manufacturing Classification System” at the conference.

IPROCOT fellows attended the 12th UK Particle Technology Forum

IPROCOT fellows, Zilin Yan (JM), Serena Schiano and Simone Loreti (UoS, Surrey) attended the 12th UK Particle Technology Forum in Manchester, on 16th -17th September 2014. They contributed an oral presentation and three poster presentations related to IPROCOT projects.

Zilin gave an oral presentation on his DEM simulation work entitled "Parameterisation of DEM Simulations: A statistical Analysis". He explained how a statistics based sensitivity analysis was performed with the DEM modelling.

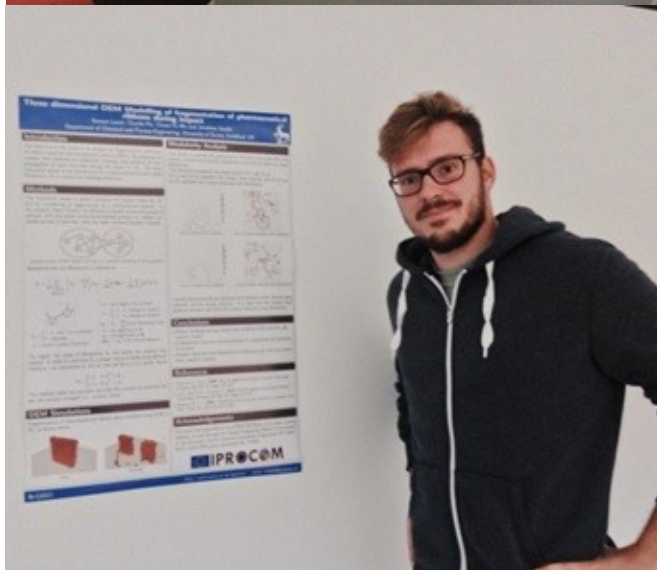
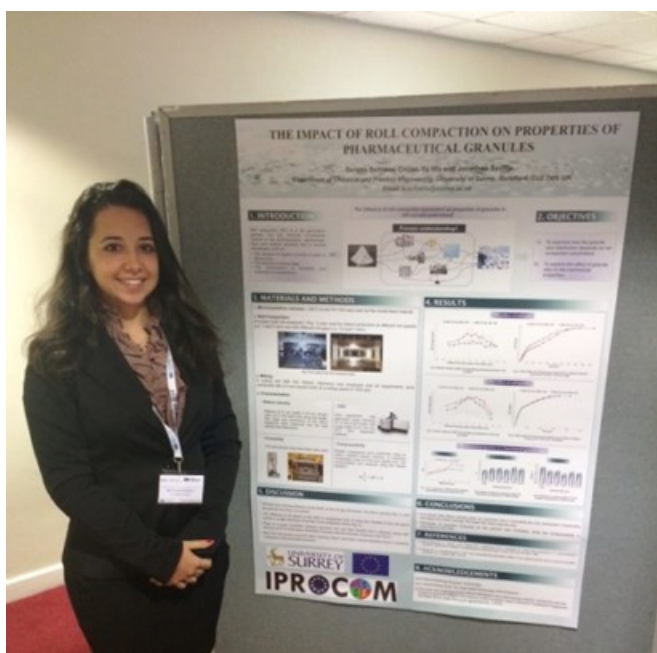
Serena Schiano presented two posters on characterizations of granular materials during roll compaction: "The impact of roll compaction on the properties of pharmaceutical granules" and "Quantification of bulk density distribution of roll-compacted ribbons using terahertz pulsed imaging".

Simone Loreti presented a poster on "DEM Modelling of fragmentation of pharmaceutical ribbons during impact".

IPROCOT Supervisor Dr. Gavin Reynolds (AstraZeneca, UK) also attended this conference as a member of the committee of the RSC Particle Characterisation Interest Group.

The Particle Technology Forum brings together researchers, and especially young researchers, active in all aspects of particle technology in the UK. This year it was held in conjunction with the international conference "Particulate System Analysis 2014". The fellows had some scientific discussions with other researchers from the two conferences working in the same areas. They enjoyed this networking and dissemination opportunity.

Serena comments: *"This was my first time to present a poster at a conference and I found it was very exciting and useful. Networking with other students, describing my work and ensuring it can be understood by others from different background were a very interesting experience. I think this experience helped me a lot in improving my communication skills. In addition, from a scientific point of view, several ideas and questions came out from these discussions that can be useful for my on-going research. I was also very impressed with the passion that so many people have for this area".*



La Fête de la Science 2014

Alon Mazor



The Science Festival “La Fête de la Science” is a French national event held since 1991 at the initiative of the Ministry of National Education, Higher Education and Research. As a free and friendly national event, the Science Festival aims to increase the awareness of the public on scientific research, and to stimulate the interests of young generation on science and technology. The Science Festival in 2014 was organized by the French department of Tarn on 26th September to 19th October, and involved 50 institutions and more than 31 actions in 20 municipalities.

As Science and its application are a dominant part of our everyday life, we believe that trying to understand the world through science is an act of citizenship. Therefore, we wish to give the entire Tarn region, large and small, initiated or not, the ability to understand the science and the world through the different actions of the Science Festival 2014.

This year, Ecole des Mines d'Albi hosted school visits in order to promote direct dialogue with researchers at their workplace and within their laboratories. Our school opened its research laboratories to high school students and middle school students from across the Tarn region and even beyond on 6th-10th October 2014. Visiting the “Science Village” allows school students to be familiar with the daily work of researchers, modern laboratory equipment and phenomena that we encounter in science and everyday life. During the event, the researchers presented their research activities and run experiment demonstrations.

As part of the science festival activities, I performed hands-on experiments for the visiting school students. The hands-on workshop called ‘Powders behaviour’ and included the following topics: interparticle space (volume), compaction of powders, interparticle forces, and mixing and segregation of powders. First, the school students were asked: “What is a researcher?” and “What are the three states of matter?” followed by numerous experiments that help them understand the behaviour of powders and their characteristics.

The Science Festival was a great success and the children became highly motivated to discover science and were very curios. This first engagement of school students with science may lead to a new generation of excellent young researchers that will push science forward.



Alon is demonstrating an experiment on interparticle forces

First Secondment Experience: From DÜSSELDORF To BERLIN

Ana Perez Gago



In the IPROCOT project, fellows like me are employed according to Marie Curie terms and conditions, in which mobility (i.e. moving to a new country) is a basic requirement. However, this is just

the first step, as part of the training programme for Marie Curie researchers, we also need to undertake “Secondment” that means to work for a short time period (weeks or a couple of months) with other partners and collaborators in their premises.

My first secondment took place during May and June 2014 at Bayer Pharma AG (Formulation Development Solids) located in Berlin. I am working on the project called “Roll compaction scale-up”, consequently, my work involves an investigation of the change in scale of the roll compactors. Therefore, the reason why I went to Bayer in Berlin was that there is the same

model roll compactor that we have in Düsseldorf, but in a larger scale. My task in Berlin was to produce ribbons and granules under different process settings in order to compare later their properties with the ones produced under the same conditions with a smaller scale compactor in Düsseldorf.

During my eight weeks in Bayer, I produced 23 different types of ribbons according to a design of experiments (DOE). Therefore, considering that I have to work with pure MCC, pure Mannitol, and 5 mixtures of them, I performed these DOEs consisting of 23 runs, a total amount of 7 times. Bayer kindly supplied me the materials as well as lab coats and personal safety equipment for working in its Formulation Development of Solids department, and I had free access to the roller compactor and any other equipment that I need. Apart from that, all the colleagues were very friendly and always willing to help, which made my time there unforgettable.

Therefore, I would like to take this opportunity to share my own experience for two purposes. First of all, I would like to encourage all my colleagues who are a bit worried of this temporary change, as this is a wonderful experience, and a rare opportunity to work outside their host institutions to learn more and discover new ways of working. Secondly, I would like to thank openly Bayer Pharma AG in Berlin for hosting me during these two months that definitely made me improve myself. Special thanks to Dr. Sarah Just and Dr. Susanne Skrabs for arranging my stay at Bayer, thanks to Christian Nienerza for teaching me how to deal with the new compactor, for all tips and for showing me that when you like what you do, your work is also a hobby. Many thanks to all these colleagues or bosses that had always a smile for me and make me feel as a member of Bayer (temporarily!): Matthias Kunze, Ataklti (Ati) Mhretab, Franziska Gromes, Stefanie Höhlich, Frank Ebel, Dr. Sven Graßmann, Dr. Adrian Funke, Dr. Anke Stroyer, Dr. Klaus Benke... and many others. Thank you for this experience!

Bayer HealthCare (Berlin) where Ana did her first secondment



Fellow of this issue



Varun

Kumar Ojha is from Kolkata, India. He received his Bachelor of Technology and Master of Technology in Computer Science & Engineering from West Bengal University of Technology. He worked as a Research Fellow in a Department of Science & Technology, Government of India funded project entitled "Development of Intelligent Recognizer for Component Analysis of Manhole Gases" hosted in collaboration of Visva Bharati University, Santinketan, India and Indian Institute of Engineering Science and Technology, Shibpur, India.

He has authored/co-authored several research articles in peer-reviewed journals and conference proceedings. He is a student Member of IEEE and Associated Computing Machinery (ACM). His research interest includes Artificial Intelligence, Machine Learning, Soft Computing, Image Processing and Pattern Recognition. His present research activity includes the advancements in Computational Intelligence and application of available Soft Computing tools for solving real life problems and the theoretical and application parts of Machine Learning algorithms.

He is presently working as an Early Stage Researcher (Marie Curie Fellow) at IT4Innovations, National Super Computing Center, VSB - Technical University of Ostrava, Czech Republic. He is exploring and studying various aspects of pharmaceutical industry for modeling the processes. As a contributor to the project he will develop a Computational Intelligence model for powder mixing process to identify critical particle properties and critical process variables that dominate bulk powder characteristics. He has conducted experiments and designed models using available computational intelligence tools to address the task of prediction/regression and identification of significant features out of a large collection of features.

He enjoys his research on the IPROCOT project. He takes the opportunity to work and interact with distinguished researchers from Academia and industry, which also helped to enhance his skills and knowledge and he is looking forward to contribute to the scientific community for the benefits of society and humanity.



Key Dates

20 October 2014

21 - 23 October 2014

23 - 27 March 2015

Mid-term Review meeting, Krakow, Poland

IPROCOT ATC3, Krakow, Poland

IPROCOT ATC5, AstraZeneca plc (AZ), Macclesfield, UK

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