MATHEGRAM Newsletter

Issue No. 5 October 2022

With only eight months remaining we are now entering the final phase of MATHEGRAM project. We have completed our Network wide training events and most all the ESRs completed their secondments, despite of the challenges and difficulties we faced during the pandemic. Our ESRs have published 16 papers from their research, well done! Please keep informing Ling about your new publications in order for her to register your paper onto MATHEGRAM research portal.

Three ESRs (Arnesh, Alex and Brayan) have already completed their projects and started their next endeavours. They will be missed and we wish them all the best in the future career.

This issue of Newsletter contains a number of interesting contributions from our ESRs, showcasing diverse activities related to MATHEGRAM. These include not only ESRs' secondment experience but also an intern's experience at SIMAP from a special guest. In addition, Ranjan (ESR2) reported an interesting outreach activity carried out at TUG. I also hope you enjoy reading the research highlights in this Newsletter.

In the past few months, we successfully organised two MATHEGRAM dissemination events in conjunction with CHOPS 2022 in Salerno in Italy and WCTP9 in Madrid, Spain. These events provided a great opportunity to showcase MATHEGRAM research to a wider international audience and they have been well received.

Prof. Charley Wu
MATHEGRAM coordinator

Inside this issue

This project has received funding from the European Commission's Marie Skłodowska-Curie innovative training Network under grant agreement No. 813202.

MATHEGRAM symposium at CHoPS 2022

MATHEGRAM symposium at WCPT9

The International Conference on Conveying and Handling of Particulate Solids (CHoPS) 2022 and Mathegram symposium

Sina Zinatlou Ajabshir (ESR 9, UNISA) and Balaji Soundararajan (ESR 11, UNISA)

The tenth edition of the International Conference on Conveying and Handling of Particulate Solids (CHoPS) 2022 along with the Mathegram symposium was conducted in Salerno, Italy from July 5th to July 9th 2022. The event was successfully organised by Prof Massimo Poletto, Prof Diego Barletta and a team of members from the University of Salerno and the Italian research community. Ever since the conference had it beginning in 1995, this conference gathers particle technology researchers and experts from all over the world. This year's theme was "New horizons for particle mechanics and solids handling in the smart manufacturing revolution" and more than 200 people participated.

The scope of the conference includes the science and technology for the production, transformation and handling of any particulate material such as but not limited to, chemicals, minerals, ceramic, pharmaceuticals, foods and health products, conventional and biomass fuels, wastes, particles for 3d-printing and includes also the mechanics of particulates relevant to environment preservation and care.

There were numerous presentations and poster sessions on diverse topics within the scope of particle technology, which were well organised and scheduled. As a part of the Mathegram symposium, a separate session chaired by Prof Charley Wu and an ESR was included, in which all the ESRs presented their research. This conference also paved way for meeting the Mathegram team in person after the advanced training course (ATC 1) held in TU Graz in November 2019. Various keynote lectures from experts from both industry and academia were also included in the conference.

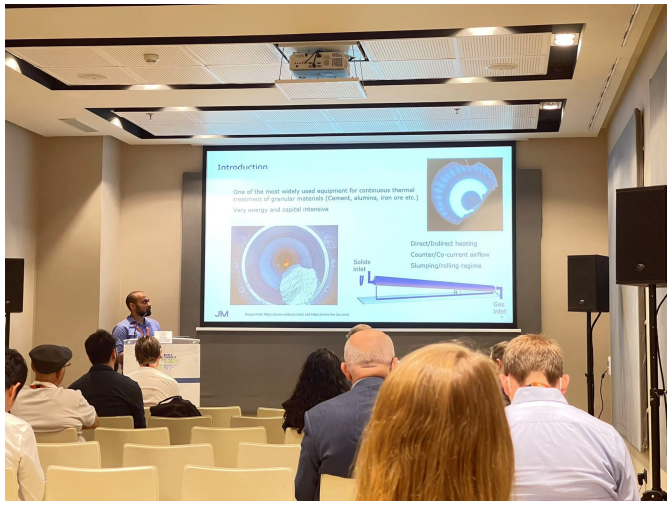
This unique forum helped in promoting the exchange of technical and scientific information in the academic and industrial sectors in the fields of solids flow, mechanical behaviour of bulk materials, powder testing, mixing and segregation, modelling, etc. It was also designed to foster business and collaboration opportunities around the world. The conference dinner was arranged at the Medieval Arechi castle, located 300 meters above the sea-level overlooking the Mediterranean coast. A guided tour was also organised to visit the Norman cathedral, archaeological museum and Paestum. A Mathegram dinner was also organised and people from the consortium had a refreshing time.

Overall, the conference was a massive success and very informative. The objectives of the conference were achieved.

The MATHEGRAM Joint Event at WCPT9

Rafael Rangel (ESR 13, CIMNE)

The 9th World Congress on Particle Technology (WCPT9) was held in Madrid, Spain, from the 18th to the 22nd of September. MATHEGRAM, of course, could not stay out of it. So a joint event, in the form of a mini-symposium, was organized where the MATHEGRAM ESRs could present their research work in oral communications. Each presentation lasted 15 minutes, including discussions, and a total of 6 presentations were given by 5 ESRs and an external guest. Unfortunately, not all ESRs could go to Madrid due to visa reason, but the great attendance showed that the interest in our projects from the particle community is very high. Some of the ESRs also presented their work in other sections, including poster and flash presentations. During the congress we had one more opportunity to meet each other in person, as well as establish good connections through fruitful discussions with many people from all over the world who are working on similar topics, whether in academia or industry. Hopefully, we will be able to meet again and further strengthen these connections at future conferences.



The IPPT's "Simulation Science"

Ranjan Dhakal (ESR2, TUG)

The IPPT's "Simulation Science" (https://ippt.tugraz.at/simSci) group, hosted the event to demonstrate: "The virtual sandbox" and "The recipe for a sand castle" – for random school participants with different background. There were children between the age group 8-16, from different schools in Graz.

The students were divided between 2 groups. Each group were around 6 participants along with their teachers from their summer campaign. One group were exhibited with the virtual sandbox while the other group with the density of sand.

We showed the Reynold's dilatancy experiment to demonstrate them what exactly happens while squeezing the mixture of water and dense granular media of glass beads. This was then followed by the ping-pong ball pyramid experiment to illustrate the role of liquid bridge. Finally, the children were given the sand materials along with the weighing device to find the bulk density of the sample with varying water content. In the end we presented the behavior of the bulk density of the sand with increasing moisture content and presented the idea for a sand castle recipe.

The kids were genuinely expressive and some of them were very curious to grasp the fundamentals. In the end they really enjoyed their time to learn the importance of bulk density.

My secondment experience at Janssen

by Domenica Braile (ESR4, UoS)

One thing I love about ITNs, such as MATHEGRAM, is the possibility offered in terms of travelling and experiences abroad. Right after my secondment in France, I headed directly to Belgium to start my three months experience in Janssen, the pharmaceutical company of Johnson & Johnson.

Janssen reception (Beerse, Belgium)

I was looking forward to starting this secondment because this would be my first experience in an industrial environment. Janssen has around 40 000 employees spread all over the world and in Beerse (Belgium) there is one of the main research & development centres, hence, I was glad to get the opportunity of working in the Oral Solid Development (OSD) department of such big company, under the supervision of Bart Nitert.

My research topic was to explore the disintegration of pharmaceutical tablets containing amorphous solid dispersions; hence, I also had the opportunity to manufacture tablets first-hand and get trained to use several pharmaceutical machines and techniques. Indeed, my experience in Janssen was formative from different perspectives, first I had the opportunity to confront my academic way of thinking with my industrial supervisors' way of doing research, which made me gain lots of skills. Moreover, being human medicines for clinical trials manufactured in their laboratories, the OSD department must follow the "good manufacturing practice", which is a series of rules to ensure a consistent high quality of the medications. Thus, to get access to their laboratories I had to be trained and abandon many habits, such as using cosmetics or wearing jewellery but experiencing such strict rules made me more conscious about contaminations, responsibilities and the safety measures which are established in the pharmaceutical industries.

During my staying in Belgium, I lived in Antwerp, the largest city of the Flemish region in which 40% of the population has a migrant background that makes the place very welcoming to foreigners. The city is famous for the Belgian chocolate, beer and art, as for example the central station which is considered the most beautiful train station in Europe and the statue "Nello and Patrasche" representing the friendship between a child and a dog.

Obviously, I enjoyed my time in Antwerp and made friendships and experiences which will always be a part of me.

Thermal Radiation & Fast Simulation - Report on BASF secondment

Jelena Macak (ESR5, DCS)

I spent three months at the end of the year 2021 doing my secondment at BASF. Each morning, I'd walk the bridges across the rivers Neckar and Rhine to get from the city of Mannheim to the city of Ludwigshafen. Then, after passing the high-security check at the gates of BASF, I'd ride a bus to my final destination, the department for computational fluid & particle dynamics. Here, I'd meet Dr. Rouven Weiler and Dr. Dominik Weis for discussions on the role of thermal radiation in industry.

Fig. 1 Industrial landscape at rivers Rhine and Neckar

Dr. Weis runs simulations of a rotary calciner. Particles processed in the calciner are miniscule, so much so that even after coarse-graining our domain holds about 75 000 parcels. A mere minute of simulated time runs for nearly a week on 8 processors. Adding a radiation model on top of it is a question of prudence. A precise model, such as Monte Carlo ray tracing, adds several calculations per particle, and would slow down the simulation immensely.

But can the radiation even reach through the dense particle packings? This question still vexes many engineers and researchers.

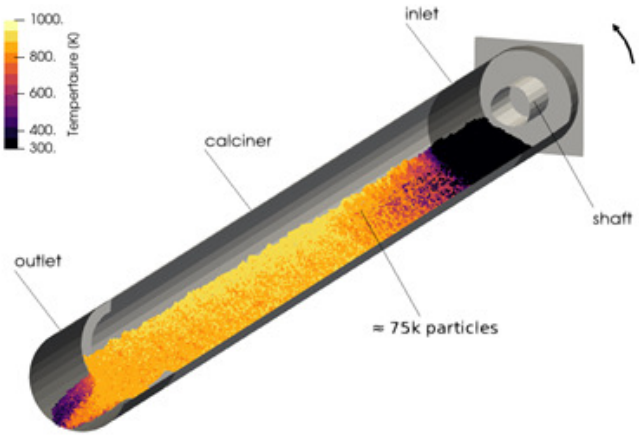


Fig. 2 Rotary calciner: electrically heated walls bring particles to 1000 K, via conductive, convective, and radiative heat transfer.

In a densely packed bed, a photon can travel only a short distance---on average, roughly 2/3 of the particle diameter (1)---before being absorbed or scattered away. This means that the majority of radiative heat from walls decays already within the first layer of particles. Modelling-wise, radiation could then just appear as a simple heat source at the granular free-surface, and be neglected in the bulk.

On the other hand, void spaces between particles act as black cavities (2): they confine the photons, leading to near-perfect absorption. Therefore, the energy that got attenuated within the first layer, will get re-emitted, and propagate via voids through the bulk.

Dr. Weiler calls this discussion "philosophical" and hands me a simple test case to show if including a radiation model will in fact change anything. The test case is a cylinder packed with consolidated graphite spheres. We impose 1500 K at the bottom, and keep the remaining walls at ambient 300 K. To shorten the waiting time, we use P1--a simple approximate radiation model.

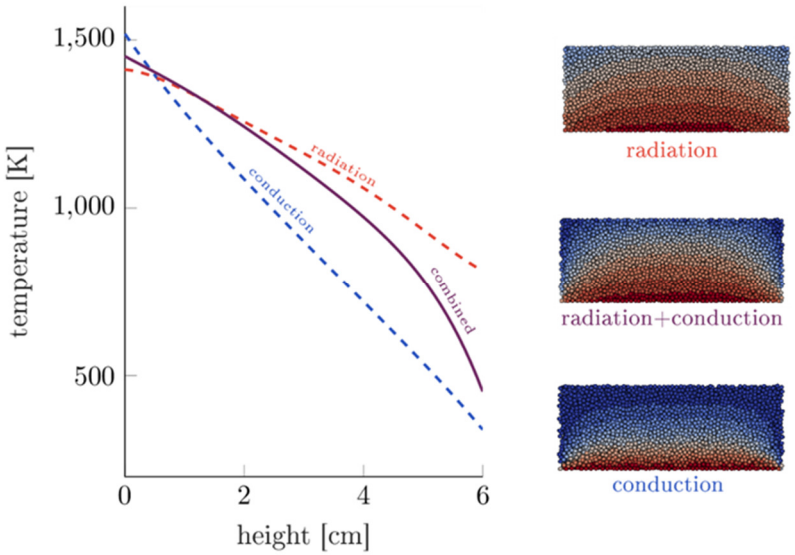


Fig. 3 Effect of radiation and conduction on the temperature distribution within a densely packed bed

The differences in the results are striking. Due to the fourth-power proportionality, radiation favors high temperatures, and in the radiation-only simulation, the whole bed is heated at above 1000K. In the conduction-only simulation, all temperatures are equally important and the distribution is linear. Joining the two modes of heat transfer yields a convex distribution curve, that is radiation-dominated near the heated wall and conduction-dominated near the cooled wall.

In the rotary calciner, though, the goal is to bring particles to a uniform temperature. There is barely any visible difference in the final state after I introduce a radiation model. However, the interaction of all heat transfer modes accelerates the changes, and the heat-up finishes quickly. Less time needs to be simulated. And while the simulation, with radiation included, still runs a week for a minute, we end up saving up some days, by skipping over some minutes.

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My internship experience in the MATHEGRAM framework

Roberto Barbano (Master's student, UNISA)

Thanks to the opportunity given by MATHEGRAM, I joined as an intern in the project involving ESR14 - Aatreya Venkatesh in February this year at the SIMaP laboratories in Grenoble, France.

The project was indeed sort of a continuation of the novel in-situ experiments on ceramic sintering at the particle-length scale carried out by Aatreya, under the supervision of Prof Didier Bouvard. Going a step further from the already realised in-situ methodologies for free sintering of alumina powders, we studied another aspect of sintering called constrained sintering - by tracking the evolution of sintering of a more complex ceramic powder mixture of zinc oxide with alumina inclusions. I must also acknowledge the support of my professor in my master's studies - Prof. Diego Barletta here, who is in fact a part of the MATHEGRAM project as well.

Prior to joining the project, my studies were focused on the theoretical aspects of design and optimization of chemical and physical processes, production processes, unit operation designs, catalyst formulation for chemical processes etc. The internship was a perfect way of seriously testing my practical skills.

On the very first day of my internship, I joined a 24-hour non-stop in-situ nano-tomography experiment at the ESRF Synchrotron. It was a crazy experience: I was so excited to spend the whole day there, but at the same time, so tired and sleepy during the night! Thanks to the experiment, 3D images were acquired with a super high-resolution of 25nm. In the following months, we used this data to study and analyze the behaviour of the zinc oxide matrix and the influence of alumina inclusions during sintering. The evolution of defects like inter-agglomerate pores and cracks formed as a result of the inclusions were analysed qualitatively and quantitatively. I also got a chance to perform dilatometry and SEM investigations.

Life in SIMaP was not limited to just experiments and simulations. I met and made friends with several PhD students and interns from different regions of the world.. Oguz, Gilmar, Brayan to name a few. They shared their life journeys, explaining me both the beautiful aspects and the difficulties encountered in the course of research. We did a lot of activities outside the lab, they gave me plenty of suggestions for my future and helped me when I was in trouble as well. It was my first time without my family in another country outside Italy. This made everything more challenging but satisfying at the same time, as I managed to deal and solve the problems by myself. In addition to having most advanced research centers such as the fourth generation Synchrotron, Grenoble offers beautiful mountains of the 'Tour de France' fame, such as Chamrousse or Alpe d'Huez.

It feels like I realized one of my dreams and I am now carrying on with my life with a lot of memories and learnings. I wish to take advantage of this amazing experience to start a new chapter in my life and career: I will try to combine the experience acquired in this internship, in materials engineering, with my background in chemical processes, to contribute further in the research field!

An approach for interpreting thermally-induced strains in granular media

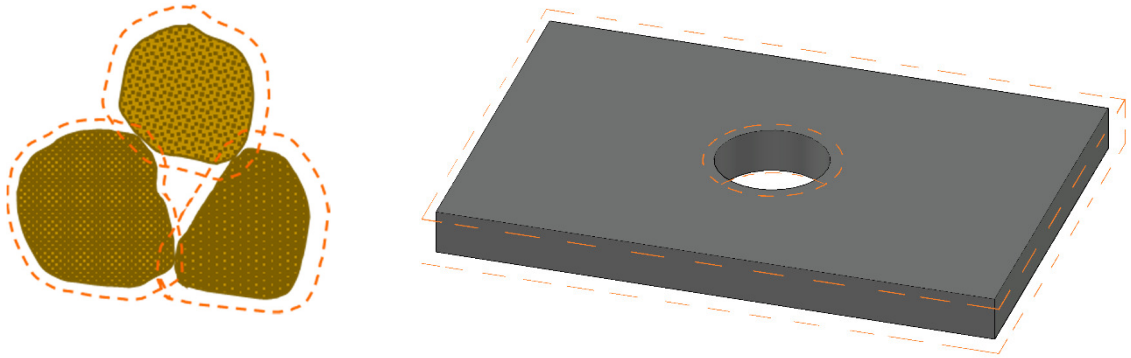
Marina Bortolotto (ESR6, IC)

The thermally-induced deformation of a granular media 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.

Expansion of individual particles (Fig. 1a) with increasing temperature is a well know phenomenon, the opposite (particle contraction) is also expected once the temperature is reduced. How much each individual particle will expand (ΔV) depends on its initial volume (V_0), the temperature change that the particle is subjected to (ΔT) and its thermal expansion coefficient that varies for different materials (α). This relationship ($\Delta V = V_0 \cdot \alpha \cdot \Delta T$) works both ways, i.e. whether temperature increases or decreases, as the temperature change can be either positive of negative.

Holes or punctures in metal slabs, for instance, will behave in a similar way (Fig. 1b). This means that holes (or void spaces) will enlarge following the same equation as presented above and will depend on the thermal expansion coefficient of the metal that the slab is made of. This means that this hole will always get bigger if the temperature change is positive.

One may wonder why voids in granular media can possibly reduce when temperature increases and the answer relies on the fundamentally different approaches used for a medium that can be assumed as continuous (metal slab) and for a particulate medium (granular soil). Moreover, granular media can be commonly associated to cohesionless materials, which means there is no binding or cementation at the contact of particles. The lack of binding allows individual particles to move or rotate with more freedom as they expand/contract, which may then lead to a reduction in voids with increasing temperature, e.g. when a particle falls towards the inside of a void.



(a) (b)

Fig 1: Thermal expansion of: (a) Individual particles; (b) a puncture in a metal slab

Whereas in discrete simulations these relative movements among particles may be more straightforward to account, it is hard to quantify them in laboratory experiments since only the overall (or bulk) response of the medium is usually measured. Therefore, assessing the changes in pore space (and hence inferring how the structure of the material has changed) requires indirect measurements and a bit of ingenuity.

It is quite common that specimens tested in triaxial cells are fully saturated. This means that all void spaces are filled with water and, as water is part of the particulate medium, it will expand or contract depending on

the temperature change. Since specimens are fully saturated, it is actually possible to quantify volumetric changes in pore spaces by only measuring the amount of water that leaves or enters the specimen during the application of thermal loads.

The initial volumes of water and solid particles are always known. Since their respective coefficients of thermal expansion are also known, it is possible to calculate the change in volume of the water (that initially filled the voids) and individual solid particles, as well as their total "new" volumes:

- Water: $V_W = V_{W,0} \cdot (1 + \alpha_W \cdot \Delta T)$
- Solid particles: $V_S = V_{S,0} \cdot (1 + \alpha_S \cdot \Delta T)$

The individual thermal expansion/contraction of the water and solid particles can be likened to an "elastic" behaviour, which means (for this context) that after a heating-cooling cycle, individual parts will regain the initial volume. The voids, however, will not necessarily demonstrate such reversible behaviour. This means that the analysis of voids requires a bit more of manipulation.

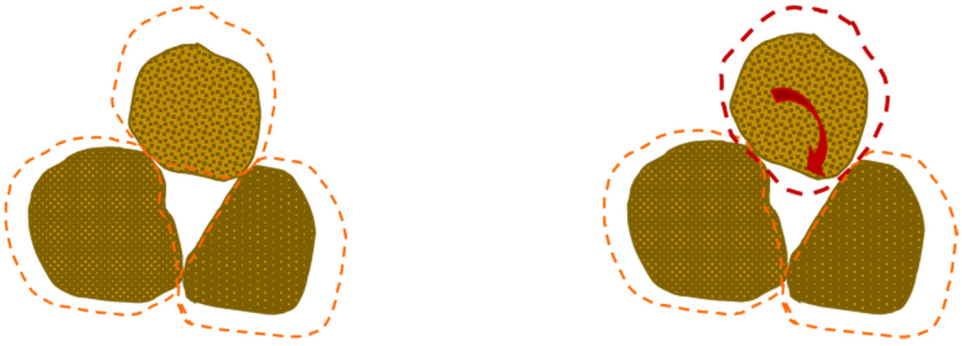
The change in voids due to a temperature change will be separated into two parts: an "elastic" portion (Fig. 2a) and a potentially non-recoverable portion (Fig. 2b). In the case of the former, the change in voids is treated in a similar way to that of the hole in a metal slab, i.e. this change in voids does not take into account any "mechanical" strain and can be calculated as indicated below using the thermal expansion coefficient of the solid particles:

- Void - "elastic" portion: $V_{V,"elast"} = V_{V,0} \cdot (1 + \alpha_S \cdot \Delta T)$

By knowing the individual thermal expansion/contraction of the water, solid particles and this hypothetical "elastic" behaviour of voids, the remaining water that is measured leaving or entering the specimen evidently correspond to the voids' (thermally-induced) mechanical strains, which are not necessarily elastic or, in other words, are not necessarily recovered once the specimen goes back to its initial temperature. The thermally-induced mechanical (TIM) strains that voids and, consequently, specimens, are subjected to can be calculated using the equation below once the volume of water that leaves or enter the specimen ($V_{drained}$) is known:

- TIM strain: $\varepsilon_m = \dfrac{V_{drained} - V_{V,0} \cdot (\alpha_W - \alpha_S) \cdot \Delta T}{V_0}$

where "V_0" is the initial (total) volume of the specimen.



(a) **(b)**

Fig 2: (a) Theoretical "elastic" thermal expansion of pores; (b) TIM strains of granular media with particle rearrangement (movement of top particle) indicated

Improving the accuracy of Pore Network Models to simulate fluid flow through sphere packings

Tokio Morimoto (ESR7, IC)

Accurate and fast methods to simulate fluid flow through granular materials are useful for studying various engineering problems related to convective mass and heat transfer, particle migration, pore water pressure rise, etc. In these numerical methods there is always trade-off between accuracy and a computational cost, where a finer mesh, i.e. better discretization of the pore space, gives higher accuracy but at a higher computational cost. Pore Network Models (PNMs) are a computational fluid dynamics (CFD) method, where individual pores are identified using the positions (and radii) of the particles and fluid flow between adjacent pores is considered (Fig. 1). The pores are the nodes in the network and the pore throats connecting individual pores are the edges. The number of degrees of freedom in PNM can be orders of magnitude less than in a CFD model where flow around particles is fully-resolved and so PNMs are computationally advantageous. However, a PNM requires a model for calculating the hydraulic conductance of the throats (edges), which act as pipes for the fluid flow. Hitherto the conductances used in PNMs have relied on empirically-based parameters and so the accuracy of existing PNMs has been unacceptably low.

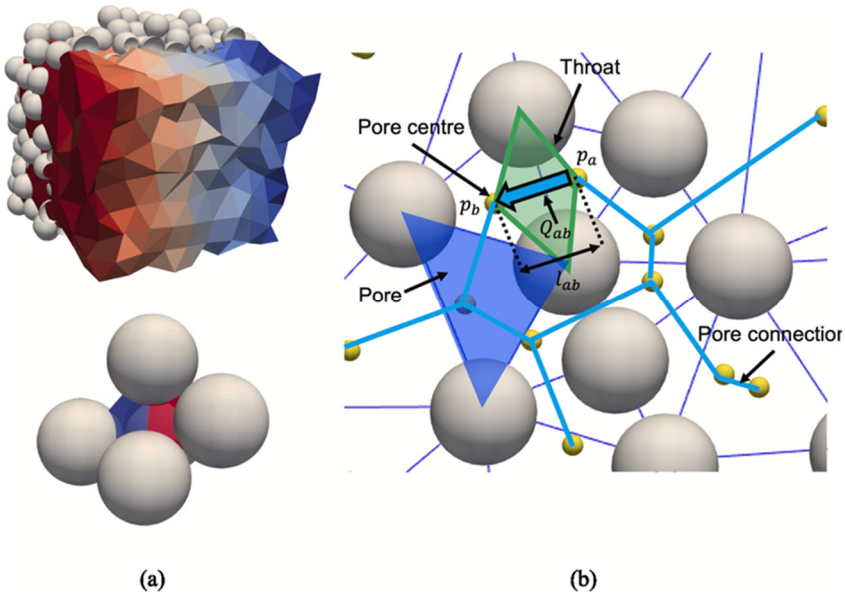


Fig 1: Thermal expansion of: (a) Individual particles; (b) a puncture in a metal slab

This study has used an analytical method to determine the hydraulic conductance of throats. The permeability of three types of lattice packings of uniform spheres (SC, BCC, and FCC) analytically obtained from Zick and Homsy (1982) was used to back-calculate the hydraulic conductance of throats in the packings (Fig. 2). The re-analysis of Zick and Homsy's analytically derived data provided a expressions for the hydraulic conductance of throats in the three types of lattice packings in terms of the packing density of the sphere packings.

The analytical hydraulic conductance expressions were implemented in a PNM, and the permeability of various random packings was calculated using a PNM with the novel model. In addition, fully-resolved CFD simulations (using the finite volume method) were conducted for the same random packings to obtain the benchmark permeability values of the random packings. A comparison between a PNM with using an existing conductance model proposed by Chareyre et al. (2012), the new analytically-based conductance models proposed here, and the fully-resolved CFD results is shown in Fig. 3. It is clear that there is a significant improvement in the accuracy of the PNM using the new expressions. This study is documented in detail in the recently published contribution by Morimoto et al. (2022).

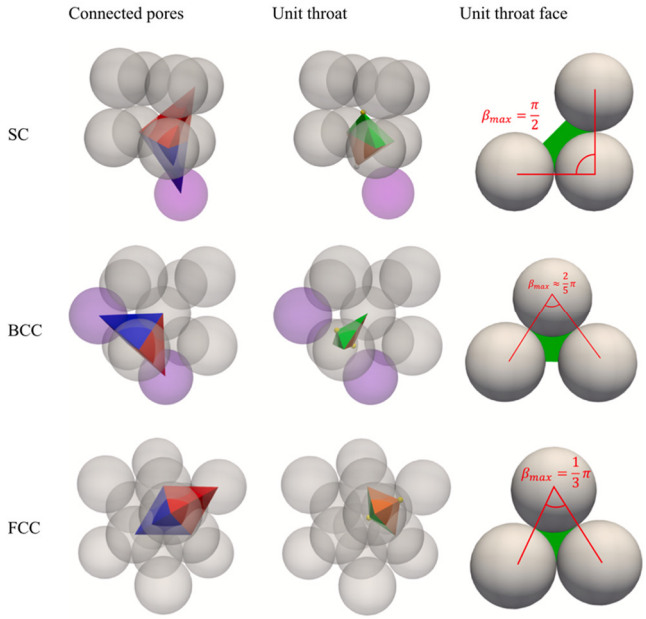


Fig 2: Schematic illustration of lattice packings and their throats. (after Morimoto et al. 2022)

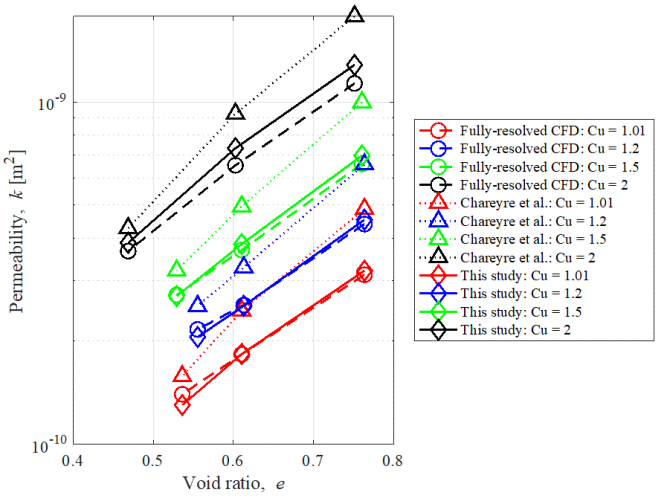


Fig 3: Comparison of global permeabilities between a fully-resolved CFD simulation and a PNM with different conductance models for random dense packings

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