MATHEGRAM Newsletter

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We are fast approaching the end of third year of the MATHEGRAM project! This year has undoubtedly been very challenging for us. Fortunately with offices, labs and country borders gradually reopening, we have been able to continue our research and training, while we are eager for our life to return to normality. I'm excited to know that MATHEGRAM ESRs have been fully engaged in research and carrying out their secondment actively. I will be delighted to read more articles on ESRs' secondment experience in the future issue of this Newsletter.

Over the last few months, we have been working closely with the Project officer at REA/EC regarding the project amendment, which has been quite a challenging and complex process. The amendment has now been approved with a 6-month Project extension, which gives us more time to consolidate our collaboration while fulfilling our project objectives.

Congratulations to MATHEGRAM fellows Marina Bortolotto (ESR6) and Tokio Morimoto (ESR7) from Imperial College, UK, for their poster presented at the British Geotechnical Association (BGA) annual conference being awarded first prize (see photo below taken at the prize ceremony). Well done, Marina and Tokio.

This year we managed to hold two consortium training events virtually: The second advanced training course (ATC2) on "Emerging applications of Granular Materials" and the Second Training School (TS2) on "Regulation, Legislation, Innovation & Collaboration". ATC2 is reported in this issue by the ESRs from the host institute. We look forward to our next training event, the third training school (TS3), which will be organised by INRAE, France. Let's hope this event can be successfully held face to face.

Prof. Charley Wu, MATHEGRAM coordinator

MATHEGRAM fellows Marina and Tokio at the prize ceremony

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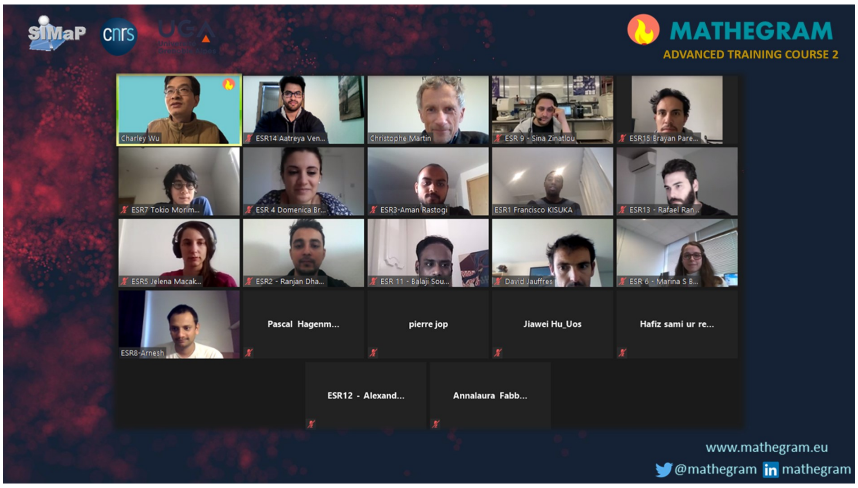
The Second MATHEGRAM Advanced Training Course (ATC2)

by Aatreya Venkatesh (ESR14) and Brayan Paredes (ESR15), SIMaP/CNRS

As a part of the series of training events planned by MATHEGRAM, the 'Advanced Training Course 2', or ATC2 in short, on 'Emerging applications of Granular Materials' was organized from the 26th till the 30th of April 2021.

Hosted by the SIMaP laboratories under CNRS in Grenoble, France, the training courses focused on the challenges and opportunities for the application of granular materials in emerging areas of materials science and were delivered by world-leading experts on the field, both from academia and industry.

As a research hub for performing X-ray tomography experiments and as the place housing the world's brightest X-ray source at the upgraded ESRF synchrotron, ideally, the event was supposed to take place face-to-face in Grenoble; but respecting the COVID-19 regulations the sessions were held virtually. Our previous experiences in handling virtual interactions within the MATHEGAM network came in handy in organizing the event. Also, social media advertisements about ATC2 on various MATHEGRAM handles led to the spread of the word and encouraged participation of many enthusiasts.



X-ray tomography, being one of the central themes of ATC2, the basics of it as well as its applications on sintering and additive manufacturing were presented in great detail by specialists from UGA, the University of Grenoble Alpes. Also, an insight into granular materials from the X-ray tomography perspective was given by professors from the Imperial college of London.

The next prime focus being sintering, its notions from a conventional sense to the more modern approaches such as laser sintering were highlighted by well-known names in the sintering field from the UGA and the University of Salerno, Italy.

Nowadays, with simulations emerging as a powerful tool to understand granular materials, specialists from UGA explained the basics and the real-world applications of discrete element and multi-particles finite element methods.

Also, staying true to MATHEGRAM's intention of bringing together industry and academia, we were exposed to lots of interesting talks from professionals of various leading companies like Johnson Matthey, Saint Gobain, Astec Industries, RCPE GmbH, Vesuvius and Ricoh 3D.

Moreover, we were treated to a keynote lecture from a research group from Clemson University, USA on developing robust processes to make high performance composite ceramic coatings. And, although we were not able to relish the beauty of snow-filled Grenoble mountains, we were introduced to a very interesting snow modeling concept from experts of Météo-France—CNRS.

Overall, considering the feedback received from the participants, we are very happy that the training event met the set expectations and objectives. It would have been all the more special if it were held amidst the capital of the Alpes, but sadly, these are the times we live in! Hopefully we get to experience an in-person training event in the near future and get to share and read about it in the next edition of the newsletter!

DEM Modelling of swelling of grains

by Domenica Braile (ESR4, UoS)

Swelling of grains is ubiquitous in many natural materials and industrial products. We can observe it at home when we place cereals in water before cooking or during industrial processes, for example the soaking of barley for beer production. This phenomenon is significant in hydrogels as well; these materials, super absorbent polymers for example, are widely used for many applications. As the swelling phenomenon usually involves a large quantity of grains, it is useful to investigate the bulk behaviour of swelling granular systems with the Discrete Element Method (DEM), a numerical method which allows to simulate particulate processes. For this purpose, a DEM model that can link the swelling of single grains with the deformation of the granular system is worth pursuing. Fig. 1 shows, as an example, the swelling of a single grain of (a) rice [1] and (b) super absorbent polymer (SAP) [2] during soaking in water. As shown in Fig. 1, the time evolution of the volume of a single grain appears to be similar for different materials. At a given external condition, the particle increases its volume (V) from the initial volume (V_0) to the equilibrium volume (V_{eq}) with certain kinetics.

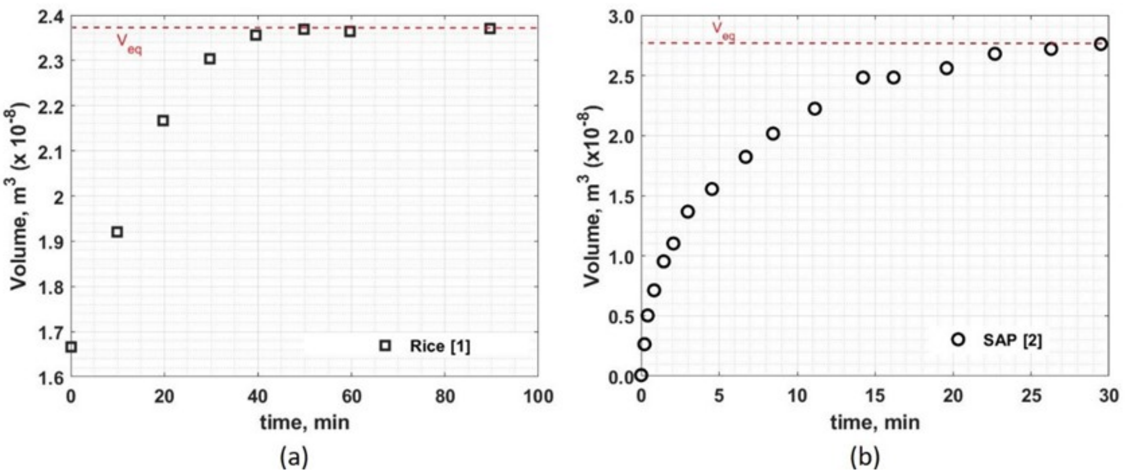


Fig 1: Swelling of a single grain of (a) rice [1] and (b) super absorbent polymer (SAP) [2]

From the experimental data, a dimensionless swelling parameter) can be defined as follows:

$$V' = \frac{V - V_0}{V_{eq} - V_0} \qquad (1)$$

and the swelling behaviour of a single grain can be approximated using a first order kinetics equation, i.e.

$$V' = 1 - exp(-kt) \qquad (2)$$

where is the soaking time and is a kinetic parameter, which can be found by fitting the experimental data for a given temperature.

In this work, the validation of the model was performed at the macroscale using experimental data for SAPs reported in Ref [2]. The swelling of SAP particles was simulated for approximately 22 minutes with the kinetic parameter k (Eq. 2) equal to 0.003 s^{-1}. Snapshots of the system at different swelling times are shown in Fig. 2 (a), while Fig. 2 (b) shows the rise of the top surface of the granular bed with time and a comparison with literature data [2].

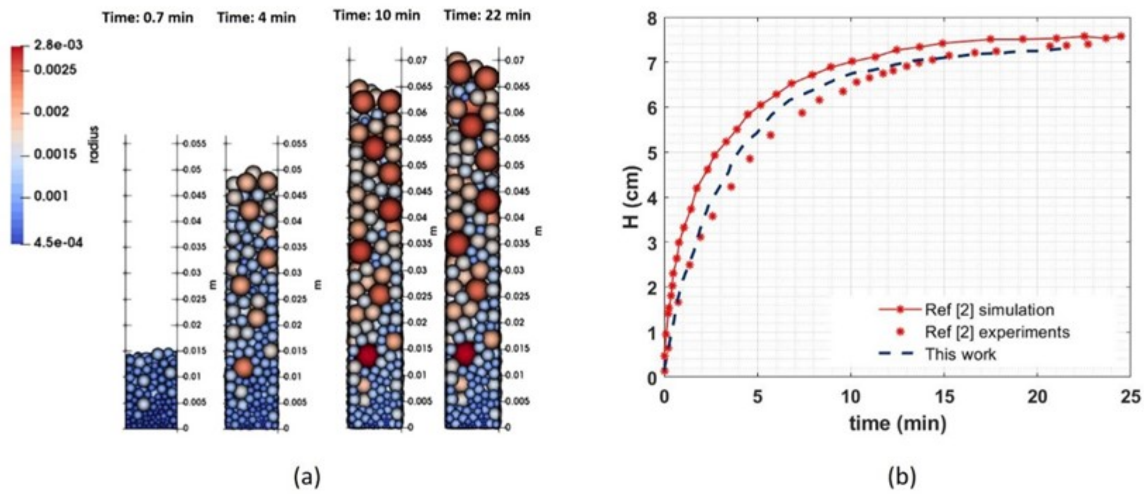


Fig 2: (a) Particle profiles at different swelling time (b) time evolution of the height (H) of the bed of SAPs

The results show that the model is able to predict the overall trend of the time evolution of the height of the bed of SAPs, however, the height is slightly overestimated between 4 and 13 min of soaking. This could be related to the assumption of a kinetic parameter (k) that is independent of the initial particle radius. Being a diffusion-controlled phenomenon, the swelling rate of each grain is affected by the initial size [3].

Future research can apply the developed model to investigate the effects of material properties on the swelling behaviour of granular media and the consequences of swelling phenomena, such as segregation, or heat generation. Moreover, the effects of the initial particle size on the swelling rate should be investigated and eventually included.

Reference

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Starch swelling at the granular scale: Granular suspensions and Rheology

by Arnesh Palanisamy (ESR8, INRAE)

Starch swelling has been a perennial subject of study for decades due to its varieties of applications and omnipresence in our everyday life. However, until now starch suspensions, during processing inside a heat exchanger, for example, have been modelled as a continuous fluid. This completely ignores the granular components of the suspensions and hence have its limitations. During a typical thermal treatment, starch undergoes a process of starch swelling called gelatinization (Figure 1a and 1b). Often in literature gelatinization is modeled at the population scale[1-6]. Only the mean size is considered and it is assumed to follow temperature-dependent kinetics. As part of this PhD, research has been undertaken to include the granular aspects and the thermal effects on rheology of such suspension systems. To realize this objective one requires a granule-scale kinetic model for swelling of starch granules.

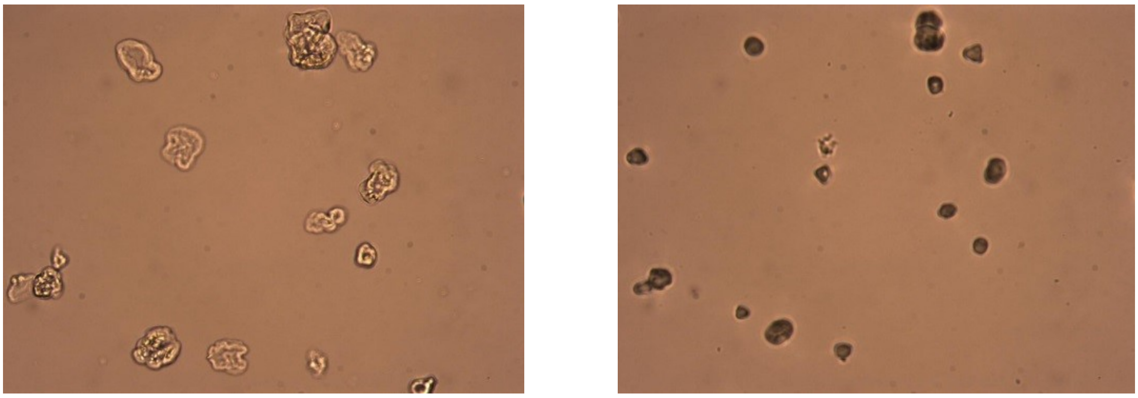

Fig 1: (a) Unswollen starch granules (b) swollen starch granules

We have performed controlled starch swelling experiments on a microscope coupled with a Linkam hot-stage to regulate the temperature. Images were captured at regular intervals and subsequently processed. This enabled collection of rich data of granules subjected to various time-temperature histories. We have used Ferret diameter evolution with time to develop a novel kinetic model for swelling of individual starch granules. This model includes a stochastic part: each granule has a random 'difficulty to swell'. First, this model was validated by comparing the predicted d10, d50 and d90 of the population as measured by the microscopy for different temperature ramps. Then, it was also validated by comparing granule size distributions measured by Malvern mastersizer after swelling under non-linear temperature evolution (Figure 2). The readers are requested to refer to our recent publication in the Journal of Food Structure[7] for further details.

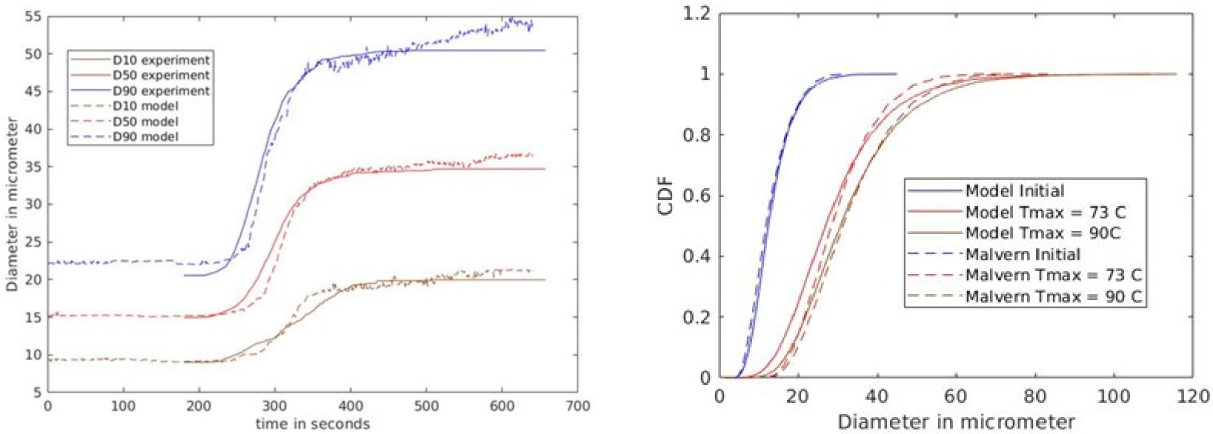

Fig 2: Model/Experiment comparison for d10, d50 and d90 and cumulative size distribution

This model has been integrated with the open-source LIGGGHTS DEM software through defining a "fix" for the same. This allows simulating the contact and lubrication interactions between granules when the sample is subjected to heating and shear, like in a heating Couette rheometer. When the granules swell, they occupy an increasing part of the available volume, so their interactions become more important which translates to an increase in apparent viscosity. This opens up avenues for utilizing CFD-DEM coupling simulations in heat exchangers where fluid-fluid, particle-particle and fluid-particle can be taken into account during thermal processing of starch-based food products. This could contribute to improvement in process control, scale-up and equipment design.

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Ranjan Dhakal - ESR2, TUG

I completed my Master's Degree in Computational Mechanics from the University of Duisburg-Essen in 2016. During my master thesis, I worked on analysis of real gas model for compressible flows. I also spent a year in Aix-Marseille University, France in 2018 where I was working on numerical modeling in fluid-structure interaction using the volume penalization method as a research assistant. Since September 2019, I started working as a Project Assistant and a PhD student at the Institute of Particle and Process Engineering under the EC-funded Horizon 2020 “Marie Curie” Innovative Training Network (MSCA-ITN) “MATHEGRAM” Project.

The aim of my present research is to investigate the thermo-mechanical behaviour of granular materials at high consolidation stresses. This can be achieved using the continuum approach (e.g. FEM, FVM) that models the detailed mechanical response. I am using "foam-extend" (an extended version of OpenFOAM which uses finite volume method) for updating and developing libraries for contact analysis. This will not only allow me to predict the behaviour of particle deformation but also practicable to couple thermal stresses with an objective to quantify and characterize the heat generation or the energy dissipated due to the contribution from inter-particle friction as well as the particle itself generating heat due to plastic deformation. Subsequently, I will continue with the novel validation which counts for the individual grain deformation against the conventional assumption where the bulk material is considered as continuum as well as with other discrete approaches.

Tokio Morimoto - ESR7, Imperial College

I am a MATHEGRAM early student researcher at Imperial College London. I was born in Japan and grew up in Mie (one of prefectures in Japan). I got my Bachelor's and Master's degrees from Civil Engineering department in the University of Tokyo, whose name is the same as my first name. In Japan, before joining this project, I was mainly researching on liquefaction of soil, which is phenomenon that soil becomes like liquid during an earthquake event. My research approach was a mix of experimental, DEM studies and some site investigations.

After living in Japan for 24 years, I decided to study abroad and fortunately, I was able to join this amazing project. I am now studying a more general topic, how granular materials like soils, food grains, and powders behave when they are heated. Now I am focusing only on DEM and working with Marina, ESR6, who is conducting laboratory experiments.

Balaji Soundararajan - ESR11

I am a PhD candidate at the department of Industrial Engineering, University of Salerno in Italy. My current research is about studying the heat transfer in selective laser sintering (SLS), which is a type of additive manufacturing technique using granular materials. My areas of interest includes engineering design, heat transfer, manufacturing and space exploration.

I obtained my bachelor's degree in Aeronautics from Anna University in India after which I worked as a Mechanical Design Engineer on Airbus A350 aircraft projects for Tata group. Later on, I moved to Berlin, Germany to pursue master's in space engineering from the Technical University of Berlin where I specialized in thermal subsystem and propulsion of spacecrafts. Before starting my PhD, I worked as a Thermal Engineer at the Centre Spatial de Liege in Belgium where I had the opportunity to work on thermal analysis of optical payloads for some of the European Space Agency's upcoming space missions. Here, I also worked on additive manufacturing of an electronic box support for Ariane 6, which sparked my interest towards this exciting research.

My current research involves both experimental and numerical investigation of heat transfer in SLS in order to establish a robust design space in terms of critical process parameters, such as laser power, laser scan speed, powder layer thickness and particle size distribution. An Infrared thermography based experimental setup has been built to measure the temperatures at the surface and also below the powder bed. Using this setup we intend to find the laser penetration into the powder bed thereby identifying the optimum layer thickness for printing. Finite Element Methods based simulations are being performed to analyse laser penetration.

I wish to utilize this learning and experience that I gain during the PhD to design and build advanced light weight structures for a sustainable aerospace industry. I also wish to 3d print habitats on the moon using lunar regolith!

Theoretical modelling of frictional heat

by Francisco Kisuka (ESR1, UoS)

Friction as a common phenomenon in daily activities can cause both desirable and undesirable effects e.g. facilitation of movement without sliding and wearing off on machine parts respectively. Such ubiquitous nature of this phenomenon has attracted a significant amount of interest from researchers of different fields.

One of the areas that has consciously received attention over the years is the area of frictional heat. Researchers have put in efforts to understand the mechanisms underlying the generation of heat from friction and the dissipation of such heat to the bulk of the body. Since the frictional heat manifests in raise in temperature, most studies focus on measuring or estimating the changes in temperature especially on the surfaces that are susceptible to friction. In this work different theoretical models for estimating the raise in contact temperature have been identified. In order to compare their robustness, these models were implemented in a simulation of two spherical particles sliding past each other (see Fig. 1). A similar set up was performed using the finite element method and the results were compared.

Fig 1: A set up of two particles sliding past each other

Results in Fig.2. show that some of these models give a very close estimations of contact temperatures. The agreement between the TK, Jaeger model and FEM model shows a very promising direction in studying the problem of frictional heat. The current step of this study is to implement the theoretical models into discrete element methods so that the study of frictional heat can be extended to granular materials.

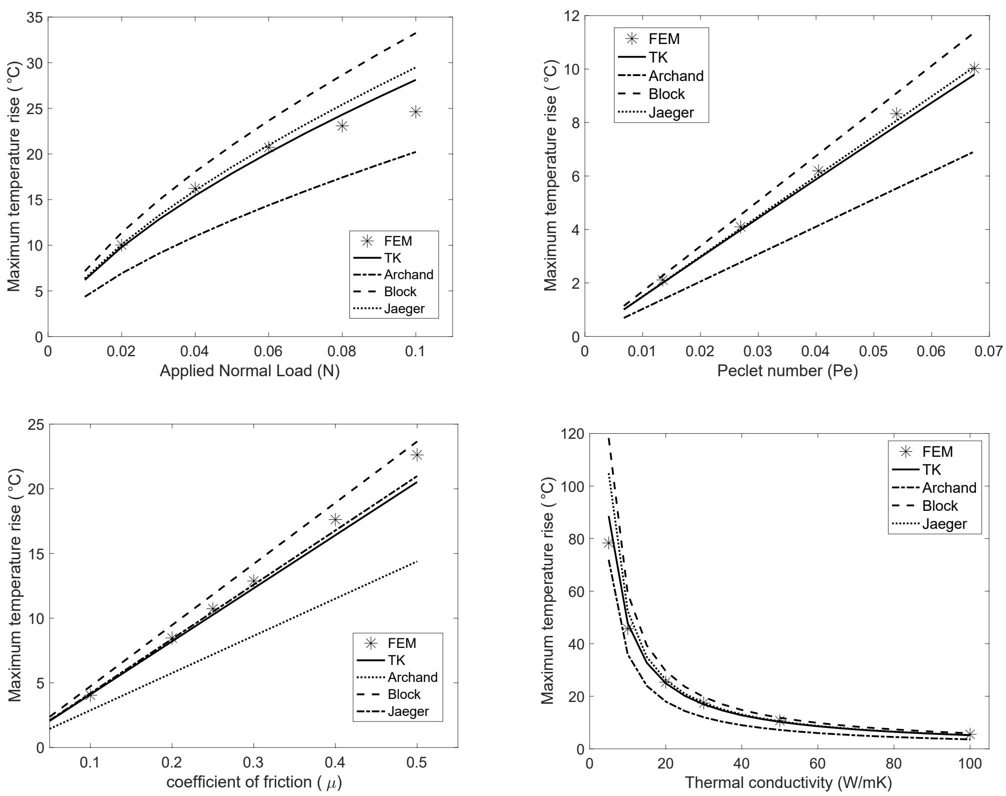

Fig 2: Prediction of contact temperature rise due to frictional heat showing TK model agreeing consistently with FEM model for varying normal load, sliding velocity and thermal conductivity

An update on infrared radiators for powder coating processes with heat sensitive substrates

by Alexandre Bobillier (ESR12, Airbus)

Powder coatings are typically coatings made of 100 % solid materials. No solvent is used in order to form a film and to cure. Unlike traditional liquid coatings, powder coatings require a source of heat to melt and flow to form a film and then a source of energy to cure. The main sources of energy used are thermal with the use of ovens or infrared radiators and radiative with the use of ultraviolet radiators.

Infrared heating is a promising technique as the wavelength of the radiation has a significant impact on the heating process. In fact, three domains of radiation are described.

- Short wave radiation, from 0.7 µm to 2 µm, tends to penetrate deeper in the material. Experimentally, such emitters are used to bring more heat in the substrate than on the upper part of the powder particles deposited onto the substrate.
- Medium wave radiation, from 2 µm to 3.2 µm, is absorbed mostly in the outer surface and predominantly heats the surface. Such radiations are particularly well absorbed by many polymers and is well converted into heat. This range of wavelength is the one to be favoured for polymeric powder coatings on sensitive substrates since it allows us to reduce the heat perceived by the bulk material of the substrate while favouring the heat absorbed by the powder particles.
- Long wave radiation, above 3.5 µm, is heating superficially the sample.

By the nature of the infrared emitters, one can adapt the curing conditions to any type of powder coatings. Moreover, it is possible to design systems to obtain a specific heating profile on the parts to be coated.

In the frame of the MATheGraM project, I am investigating on the usage of Carbon Infrared Radiators producing medium wave radiation for polymeric powder coatings. The results are promising since the heating and curing of the coatings can be completed in less than 2 minutes and the substrates tend not to heat above 120 ºC for powder coatings curing at 140 ºC. Infrared radiators seem to be a promising technique to cure powder coatings on heat sensitive substrates.

For more information, please contact

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