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14. ABSTRACT

The colloidal droplet spreading on and sorption into a porous medium is important to 3D printing technology. In this study, we conducted numerical simulation to investigate droplet spreading on and sorption into a powder bed and performed experiment to study the colloidal fluid distribution in the porous structure after sorption of single/multiple droplets in powder beds. The spreading of the droplet on the surface of the porous matrix is modeled based on the Navier-Stokes equation while the liquid sorption in the porous matrix is described using the

15. SUBJECT TERMS

colloidal droplet, droplet impact and sorption, 3D printing, microCT imaging

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Report Title

Final Report: Computational Study of Colloidal Droplet Interactions with Three Dimensional Structures

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Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

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TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

05/18/2015 1.00 Timothy munuhe, Alex LeBurn, Kevin Li, Liang Zhu, Ronghui Ma. Numerical and experimental study of colloidal droplet impact and sorption in porous substrate,
Thermal and Fluids Engineering Summer Conference. 09-AUG-15, . : ,

TOTAL: 1

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Timothy Munuhe	0.75	
FTE Equivalent:	**0.75**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Ronghui Ma	0.10	
Liang Zhu	0.05	
FTE Equivalent:	**0.15**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

We propose to study the dynamics of colloidal binder interactions with three-dimensional powder bed for 3DP process. The main research goals of this proposal are to (a) create a novel multiphysics model that enables the prediction of colloidal droplet interactions with complex porous structures; (b) advance the understanding of the colloidal droplet spreading, droplet sorption, and particle deposition in a porous substructure.

The research endeavor has focused on theoretical and experimental study of a ferrofluid droplet impact on and sorption into a porous powder bed. The research activities are summarized as follows:
(1) We developed a numerical tool based on the meshless SPH method for droplet impact on and sorption into a powder bed considering free surface flow above the powder bed surface, infiltration of the liquid in the porous matrix, and the interfacial forces on the free moving surface. The model has been used to study the effect of impact velocity, permeability of the powder bed, and droplet viscosity on the lateral spreading diameter and penetration depth.
(2) A model for the transport and deposition of nanoparticles in the porous matrix during droplet sorption was developed to study the distribution of nanoparticles. We developed a particle trajectory model that considers nanoparticle interaction with the porous matrix for various operational conditions including porosity, surface potential, and local fluid velocity. The trajectories of the particles and their interactions with a surface are predicted by the forces acting on the particle including Brownian motion, London-van der Waals attraction, electrostatic double layer force, buoyancy force, lift and viscous forces.
(3) The trajectory model was integrated with the meshless droplet impact model to enable a multi-scale simulation of the convection, diffusion, and deposition of the ferrofluid in the powder bed. The multi-scale modeling enables one to determine the particle concentration distribution in the powder bed after droplet sorption.
(4) An experimental study was conducted to investigate the distribution of ferrofluid in the porous structure after the droplet was absorbed using microCT scans. The powder bed consists of PMMA microparticles with particle diameters in the range of 53 - 63 μm and 125-135 μm. MicroCT scans were used to reveal the shapes of the liquid distribution after single-droplet and multi-droplet sorption in the different powder beds.

Summary of Research Findings:
(1) Through the numerical study of a droplet impact on and sorption into the powder bed, we have identified several parameters that affect the lateral spreading and penetration of the liquid in the powder bed. These parameters are the permeability of the powder bed, impact velocity, and the viscosity of the liquid.
Theoretically, a high permeability facilitates the liquid transport in all the directions in the powder. In the study of droplet sorption in the powder bed, it is found that a greater permeability causes a smaller spreading diameter and a larger penetration depth, as shown in Figure 1. It also takes less time for the droplet to be absorbed.
Our simulation results also reveal that a high speed droplet impacting the porous medium will experience a larger lateral spreading (Figure 2).
Fluid viscosity resists the droplet spreading above the surface and sorption in the powder bed. Our simulation shows the fluid viscosity affects the sorption to a larger extent than the spreading. As a result, higher viscosity fluids encounter more spreading and less sorption (Figure 3)
(2) The study of the trajectories of nanoparticles near a solid sphere reveals that the rate of particle deposition on the solid matrix decreases with a larger nanoparticle size, a higher local velocity, a larger porosity, and a larger repulsive surface potential. The simulation results are shown in Figures 4-5 in Appendix.
(3) The multiscale study of colloidal droplet sorption in the porous powder bed shows that the nanoparticle distribution in not uniform. Due to nanoparticle deposition on the surface of the powder surfaces, most nanoparticles concentrate near the top surface of the powder bed as shown in Figure 6.
(4) MicroCT images of the powder beds after single/multiple-droplet sorption clearly reveal the distributions of the ferrofluid in the porous matrix. As ferrofluid does not wet the PMMS material well, the capillary force at the flow front opposes the infiltration of the liquid in the powder bed. As a result, the distributions of the ferrofluid in the powder bed are observed to be quasi-steady state. This feature allows the usage of microCT to study ferrofluid distribution after droplet sorption. In the microCT image of the powder after the sorption of a droplet, there exists a sharp contrast in grayscale values between the regions filled with the liquid and the air, which clearly indicates the liquid front. The resultant distributions of ferrofluid can be used for model verification in the future.
All the droplets were fully absorbed and the fluid distributions in the powder resemble the shape of a truncated sphere. Despite the different powder particle size (53-63 μm and 125 – 135 μm) of the powder bed, the shapes of the liquid distribution in the powder after single-droplet sorption are close to each other (Figures 9-10, 12), with a slightly wider droplet profile for the 53-63 μm particle powder bed. The three-droplet sorption in the powder bed of particles with their sizes in the range of 53-63 μm generates a larger volume of similar shape.
Based on our previous study of microCT imaging of nanofluid distribution after injection in tissue, the gray scale value of the microCT image can be translated to local density. In the three images, the highest grayscale values are observed at the boundary of the liquid. This might be the result of compaction of the powder particles under the drag and capillary force at the flow front. Another explanation may be due to the artifact of the microCT imaging algorithm at the boundary. The cause of the high grayscale value at the boundary will be investigated in the future.
(5) Comparison of numerical simulation with microCT images
The simulation results of liquid distribution in the powder bed (Figure 6) show a wider lateral spreading than the microCT

images (Figures 9-11). The difference can be attributed to the displacement of the surface powder that was observed during the droplet impact process. The surface powder displacement forms a crater on the surface that limits the lateral spreading of the droplet. The change in the surface topography, which was not considered in this study, will be considered in future study.

Appendix 1 Figures

Technology Transfer

Computational Study of Colloidal Droplet Interactions with Three Dimensional Structures

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Appendix 1 Figures

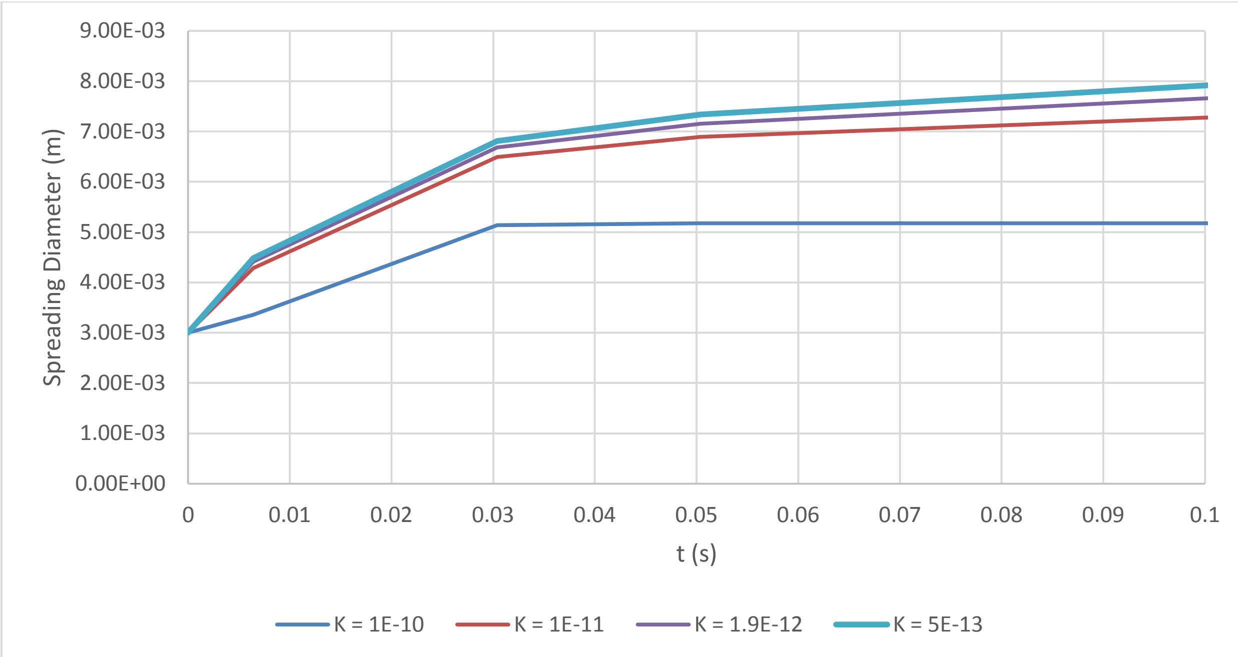


Figure 1 Droplet spreading diameter vs. time at different permeabilities (ε = 0.35, U_{imp} = 16cm/s)

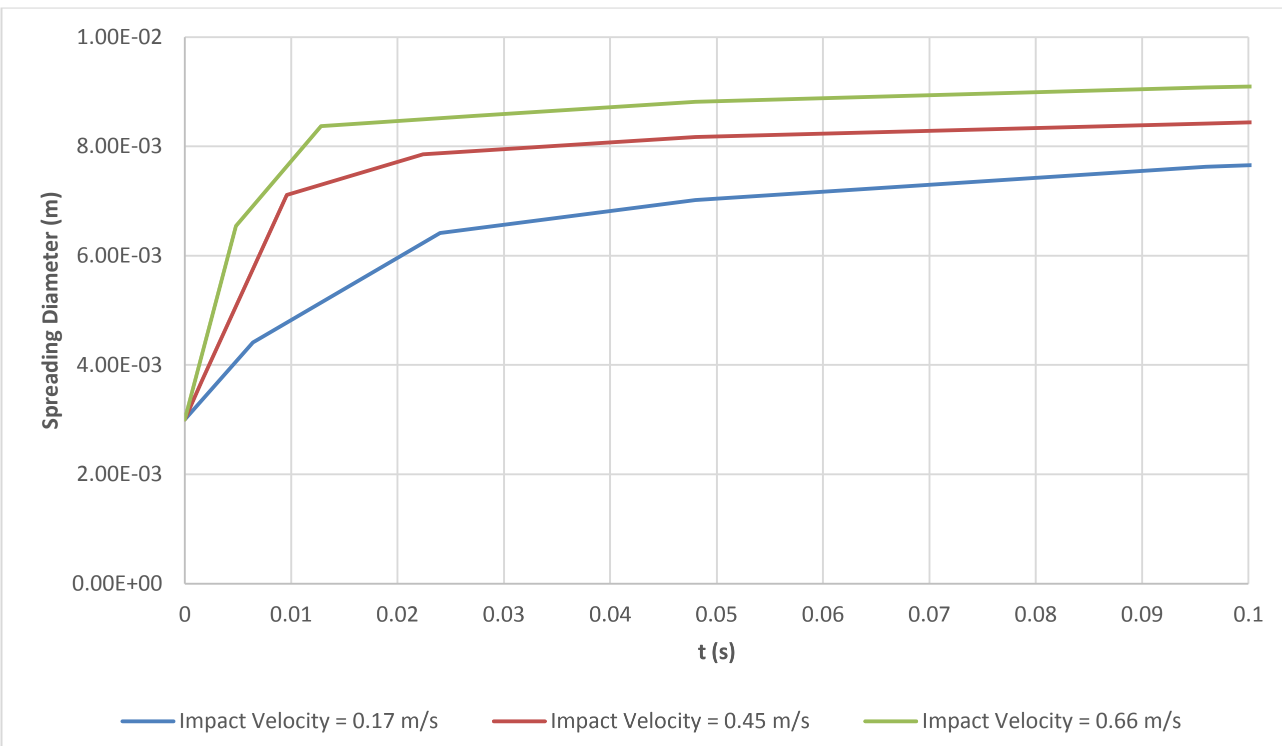


Figure 2 Droplet spreading diameter vs. time for various impact velocities using K = 1.9E-12, ε = 0.35

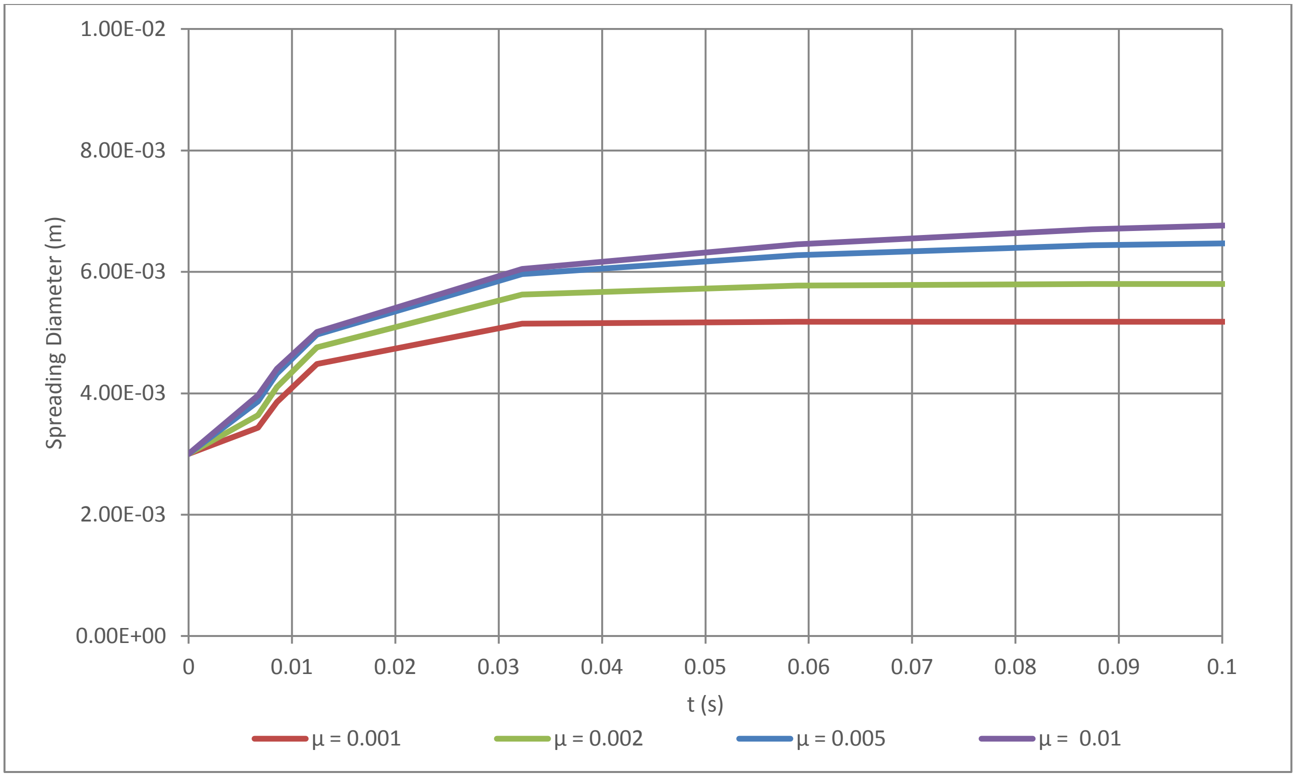


Figure 3 Droplet spreading vs. Time for various viscosities using K = 1E-10, $\varepsilon = 0.4$, $U_{imp} = 7$ cm/s

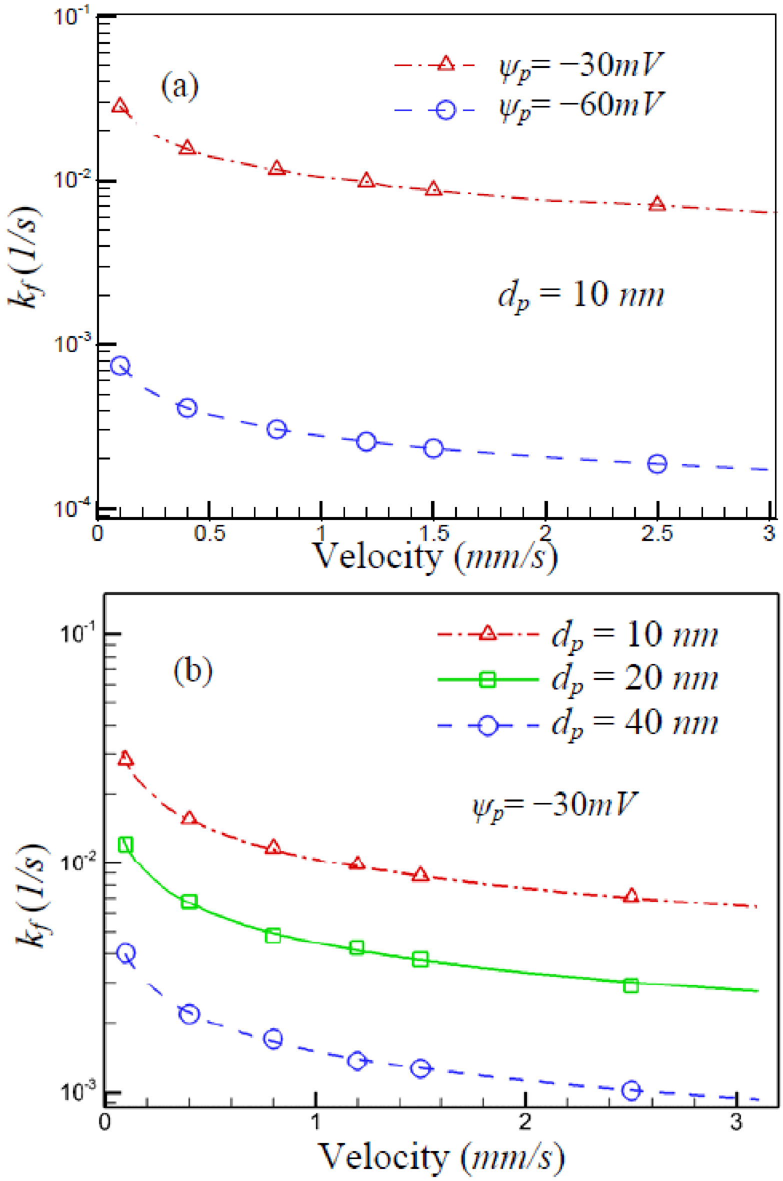


Figure 4 Variations of deposition rate coefficient k_f with velocity for (a) various negative surface charges of the particles (b) various nanoparticle sizes.

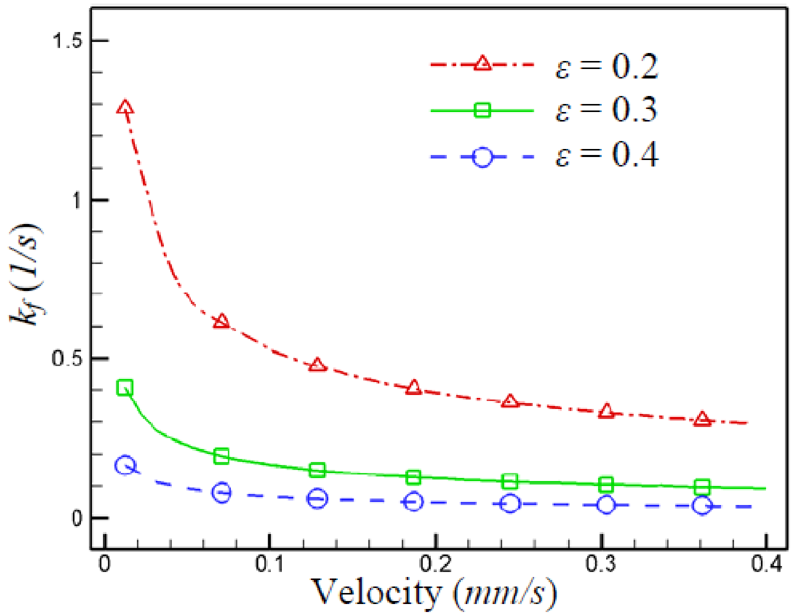
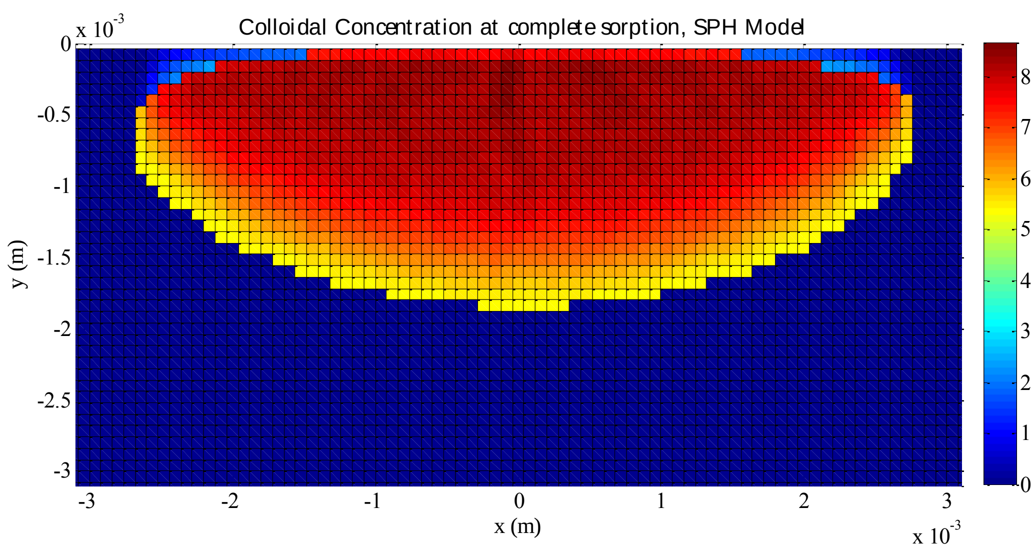
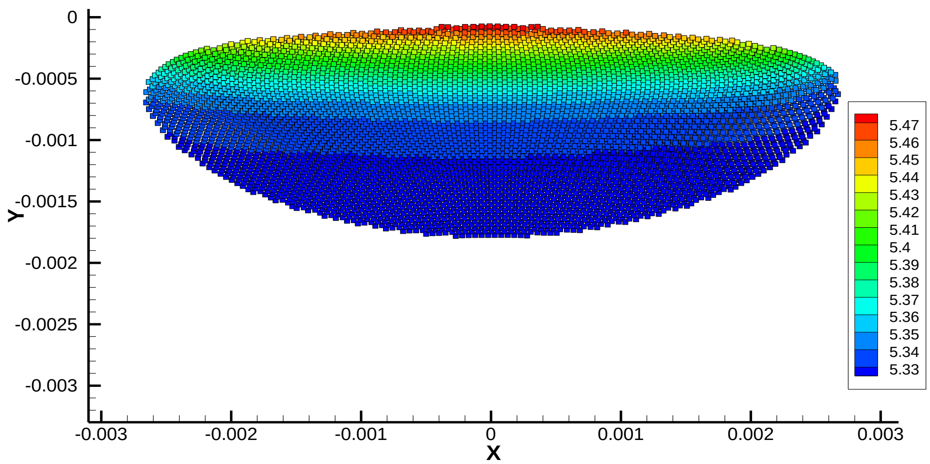


Figure 5 Variations of the deposition rate coefficient k_f with interstitial fluid velocity for various tissue porosities (ψ_c = –20 mV, ψ_p = – 20 mV, d_p = 20 nm).



(a)



(b)

Figure 6 Colloidal concentration in units of mol/m^3 of fluid and porous matrix together (a) and just fluid (b) after complete sorption in SPH model using K = 1E-10, ε = 0.4, U_{imp} = 7 cm/s

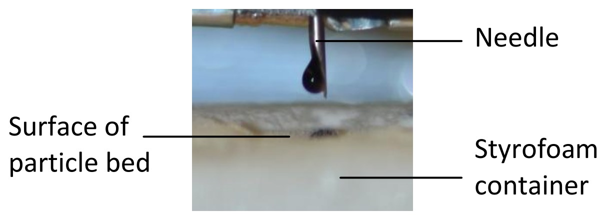


Figure 7 Set-up for droplet impact on the porous powder bed.

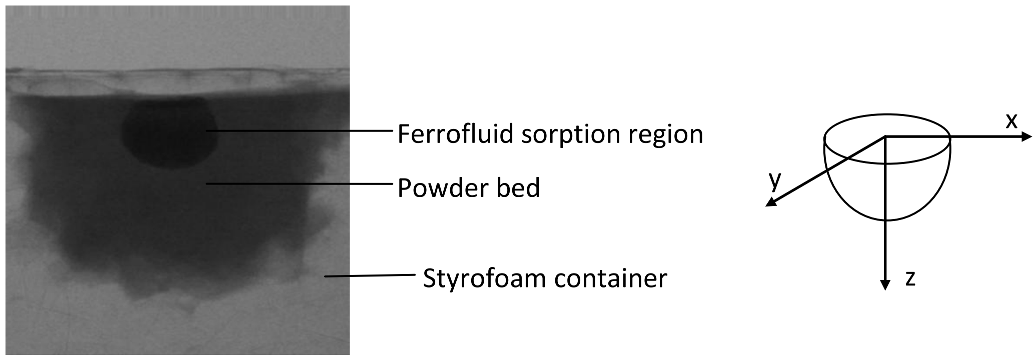
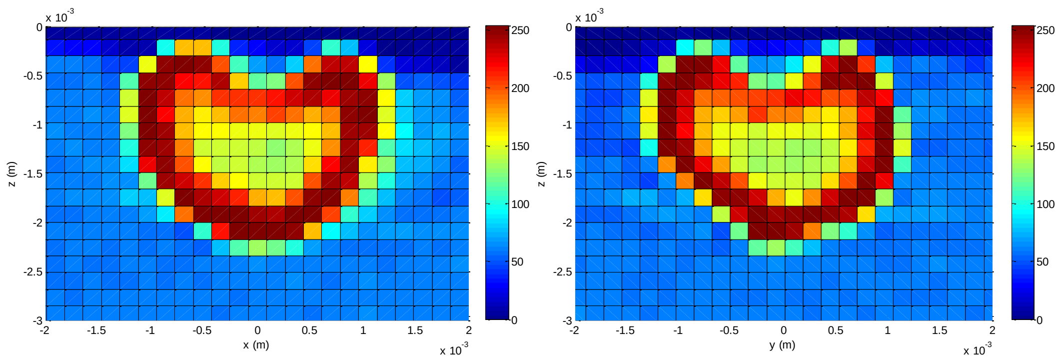
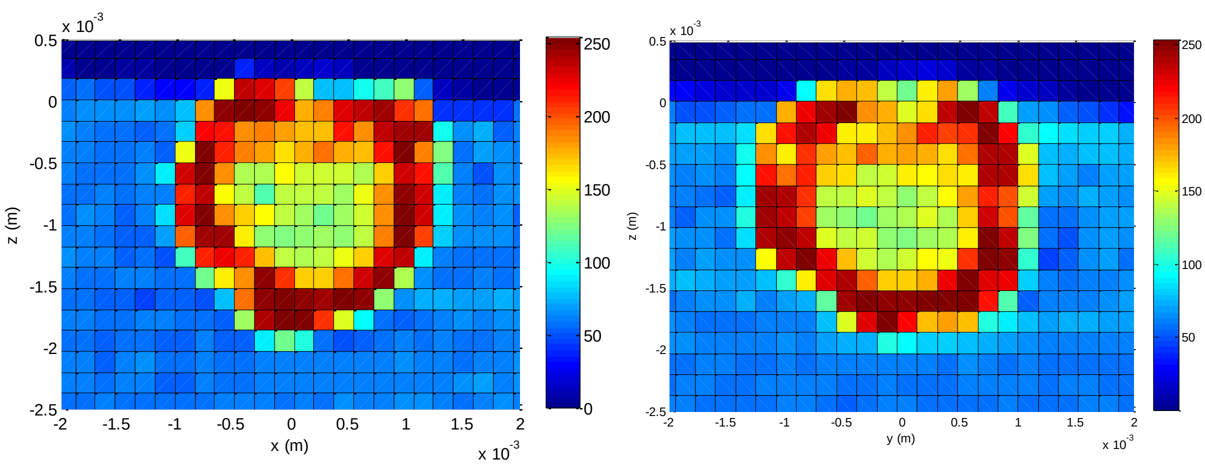


Figure 8 A sideview of MicroCT scan of powder bed after three droplets are absorbed.



(a) (b)

Figure 9 Grayscale value at (a) xz plane and (b) yz plane, 53 µm – 63 µm particles



(a) (b)

Figure 10 Grayscale value at (a) xz plane and (b) yz plane, 125 µm – 135 µm particles

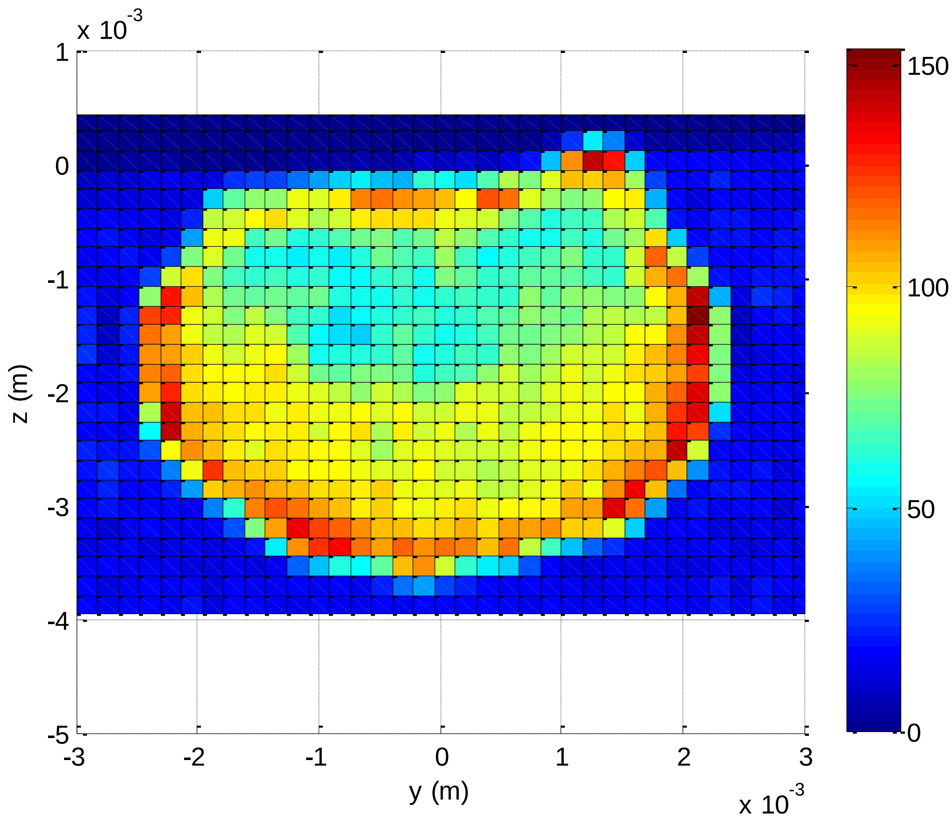


Figure 11 Triple-droplet grayscale for 53-63 μm particles

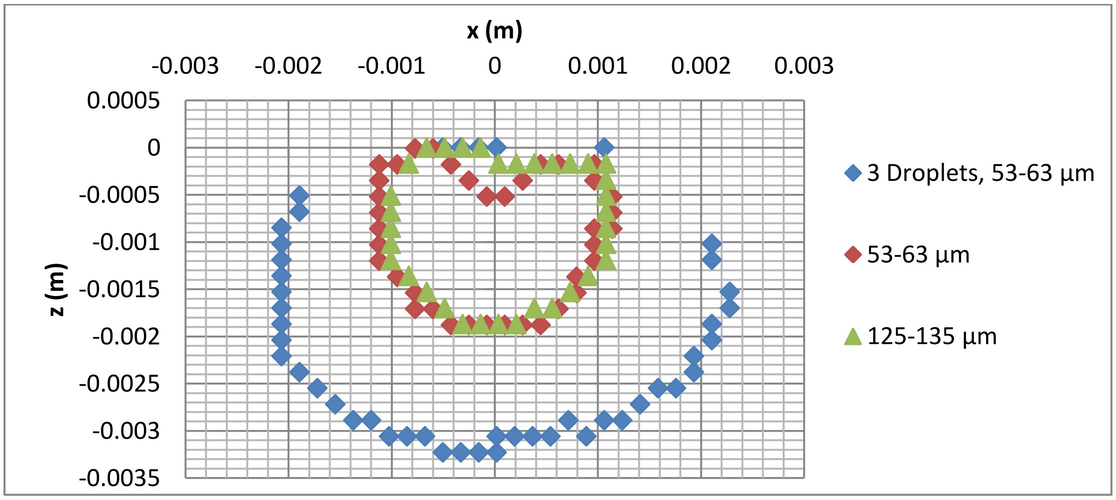


Figure 12. Droplet boundary profiles for microCT scans