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1	Study of the evolution of transport properties induced by additive processing sand mold
2	using X-ray computed tomography
3	
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#### 22 Abstract

Accurate characterization of the mass transport properties of additively processed sand molds 23 is essential in order to achieve reproducibility of the produced castings and control of gas 24 defects in foundry industries. The present work highlights the potential use of X-ray micro-25 computed tomography (µ-CT) to characterize the evolution of permeability and some major 26 microstructural features of such additively processed sand molds. The evolution of mass 27 transport properties of sand mold samples under specific processing conditions met in 28 additive manufacturing and its influence on the porosity, the permeability, the tortuosity, and 29 the pore and throat size distributions were characterized from 3D images provided by X-Ray 30 µ-CT. The obtained results showed that the mass transport properties of additively processed 31 sand molds can be closely predicted by using non-destructive in situ methods, such that 32 33 improvements to the casting can be made to create more optimized 3D printed structures for foundry applications. 34

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*Keywords:* Additive manufacturing; 3D-printed casting sand mold; Permeability; Pore Size
Distribution; X-ray μ-CT; Numerical simulations; Pore network modeling.

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#### 39 1. Introduction

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Three-Dimensional Printing (3DP) technology, also termed as Additive Processing (AP) or joining technology, emerged as a new rapid manufacturing method in foundry industries to build three-dimensional (3D) sand molds directly from Computer-Aided Design (CAD) models in layers. As compared with the traditional conventional sand mold, (Sachs et al., 1990) stated that this kind of rapid-prototyping technique offers the ability to efficiently

manufacture sand molds and cores in casting industry with optimized geometries as designed 46 with CAD without the need of extensive molding. Additively processed sand mold is also 47 advantageous over conventional methods due to its ability to reduce surface defects in the 48 molds as shown by (Hawaldar and Zhang, 2018). Rapid prototyping technique has been 49 accepted extensively in the casting industries due to its proven capability to reproduce a 50 virtually complex designed object into a real casting mold. (Almaghariz, 2015) studied the 51 economic advantage of 3DP technology and found that there is no influence of part 52 complexity on the manufacturing costs of molds and cores. This technique allows the 53 production of highly complex components in a cost-effective way as shown by (Almaghariz et 54 al., 2016) and good surface finish as shown by (Hawaldar and Zhang, 2018). Despite being 55 still limited in number, the applications of AP technique are much diversified, including 56 aerospace, automobile, and medical industries. Consequently, 3DP represents a step forward 57 58 towards autonomous casting in which a sand mold can be printed without any machining stage. In this regard, (Upadhyay et al., 2017) published an extensive literature review 59 elsewhere, so only the key features of additively processed sand molds are reminded in the 60 present article. 61

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AP has enabled the casting industries and foundries to produce more complex sand molds 63 without using any kind of physical model, through a succession of thin layer which are 64 directly generated from 3D CAD files. The layer-based rapid prototyping technology, or 65 Powder Binder Jetting (PBJ), consists in bonding individual particles with a liquid resin 66 binder, which generates porous parts. The existence of such porosity is necessary in casting 67 sand molds so that the gases can be efficiently evacuated from the mold cavity through the 68 interstices during filling of the mold. This minimizes the risk of casting defects caused by gas 69 trapping in the liquid alloy. Fig. 1(a) describes the PBJ process, in which ceramics kind of 70

materials are generally used as to provide refractoriness to the mold, and a liquid resin binder 71 provides cohesion in between such ceramic particles by forming capillary bridges, Fig. 1(b). 72 For metal casting, a temperature-resistant material is required, so silica sand is generally used 73 as granular material for the PBJ process, and a furan resin is commonly taken as a liquid 74 binder due its high performance in terms of dimensional accuracy and mechanical strength of 75 the printed mold. Also, various 3D printing process parameters directly affect the quality of 76 the sand mold. In particular, the relationship between the printing process parameters (print 77 position/orientation in job-box, recoater speed, and print resolution) and their influence on the 78 properties of the 3DP sand mold have been extensively investigated in previous works using 79 both mathematical modelling by (Coniglio et al., 2017) and experimental validations by 80 (Sivarupan et al., 2017). (Sivarupan et al., 2017) showed how the printing processing 81 parameters affected mechanical properties in 3DP sand mold. It was also reported by (Mitra et 82 83 al., 2019) that the mechanical strength and permeability of 3DP sand molds are deeply dependent on the amount of binder and the ageing conditions. In this regard, the evolution of 84 85 permeability and mechanical strength of such additively processed silica sand molds during curing was studied in a recent work by (Mitra et al., 2018) for different binder contents and 86 curing parameters, showing that the 3D printed sand molds could be stored for long time at 87 room temperature before being used for metal casting, while no substantial variation in 88 strength of 3DP mold was observed below 100 °C, the gas permeability was found to decrease 89 with increase in curing temperature. However it is of equal importance for morphological 90 characterization of such additively processed porous structures to be standardized in foundry 91 92 with proven quality control, especially as the 3DP structures can be customized and changed (based on printing process parameters) easily to alter its mass transport properties based on 93 casting requirements. 94



95

96 Fig. 1. The PBJ process showing, (a) the initial distribution of furan binder within the silica 97 sand particles, (b) the drying stage of resin-bridges by infrared heating during the printing of 98 the mold and the optional curing stage to obtain stronger resin-bridge after printing of the 99 mold.

Characterization of mass transport properties through pore networks with complex geometry 101 and connectivity, such as 3DP sand molds, is essential in order to assess the risks of 102 incomplete filling and gas porosity in castings. The fundamental microstructural 103 104 characteristics include grain size distribution, pore size distribution, throat (pore constriction) size distribution, pore-to-throat size ratio, pore connectivity, and tortuosity. These 105 microscopic physical properties will control the macroscopic characteristics of the 3DP molds 106 in terms of permeability and porosity governing the flow of liquid metal, and, more generally, 107 the heat and mass transport within the 3DP sand mold. Therefore, knowledge of the 108 relationships of 3DP process parameters and these microscopic characteristics is of vital 109 110 importance to predict casting defects. On this subject, it was stated earlier by (Sivarupan et al., 2017) that high reacoater speeds lead to lower grain packing densities in 3DP molds (porosity 111 112 depends on recoating speed). It is also known that high levels of sand compaction reduce permeability due to the decrease in volume available for fluid flow and the increase in specific 113 surface of the interstices. Pore Network Modelling (PNM) offers a simple demonstration of 114

the complex pore structure and topology, but quiet more accurate than traditional bundle-of-115 capillaries model. In PNM the void phase is divided into a set of spherical pores connected by 116 cylindrical throats. A complete review of PNM for porous geometries (pore network 117 construction) has been studied elsewhere by (Xiong et al., 2016). (Huang et al., 2019) used 118 PNM to extract the network of pores and the connected throats from a fibrous material to 119 simulate two-phase flow. It was shown by (Degruyter et al., 2009) and (Degruyter et al., 120 2010) that the permeability can be predicted using the throat size distributions with the 121 modified Archie's law. 122

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In the industrial foundry processes, numerical simulations of mold filling and casting 124 125 solidification are employed in order to optimize the part designs, reduce the manufacturing costs and prevent defect generation. However, the lack of accurate estimations of key inputs, 126 e.g., local porosity, density, permeability, and strength, limits the usefulness of the obtained 127 numerical results. Therefore, it is crucial to develop a non-destructive method to properly 128 characterize 3DP sand molds in order to predict the relationships between process parameters 129 and the inputs to such simulations. Other non-destructive methods include the traditional 130 permeability test in which air is injected to the 3D printed sample (although they need 131 132 sampling of the mold). Also, Scanning Electron Microscope (SEM) imaging could be considered as a suitable non-destructive method, but only 2D microstructural information can 133 be extracted. Although Mercury Intrusion Porosimetry (MIP) is by far the most popular 134 method for characterizing the pore size distribution of porous materials with pores in the 135 range of 500 µm to 3.5 nm as stated by (Giesche, 2006), MIP experiments are not expected to 136 work well on unconsolidated materials like 3D printed casting sands because the applied 137 pressure damages the material and its void-structure. X-ray micro computed tomography (µ-138 CT) is a non-destructive and non-intrusive method as stated by (FLANNERY et al., 1987), 139

allowing the characterization of 3D printed sand mold specimens. On this regard, a complete review of X-ray  $\mu$ -CT and its applications has been studied elsewhere by (De Chiffre et al., 2014). X-ray  $\mu$ -CT has emerged as a powerful nondestructive technique (NDT) for the direct 3D characterization of complex porous geometries. (Hazlett, 1995) stated that the 3D images of the pore space, like those provided by X-ray  $\mu$ -CT, can be used for direct computation of multiphase fluid flow and to reliably characterize permeability from the realistic digital images provided by this technique.

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Different numerical methods exist for the simulation of creeping flow through porous media 148 149 at the microscale, e.g., Finite Volume Method (FVM) and Lattice Boltzmann Method (LBM). 150 (Jaganathan et al., 2008) used FVM to model fluid flow through the real microstructure of a fibrous mat to predict the permeability and compared them to various analytical expressions. 151 (Soulaine, 2015) used FVM to perform a direct numerical simulation of fluid flow in a fully 152 saturated porous media for the prediction of permeability from µ-CT image. (Thabet and 153 Straatman, 2018) idealized a geometrical introduced to characterize small volume of packed 154 sand in pore-level computations using YADE (Yet Another Development Engine) solver. In 155 previous research by (Boek and Venturoli, 2010), it was proved that using LBM, to obtain 156 permeability from a digital image is a reliable alternative to destructive traditional 157 measurements. (Malaspinas et al., 2010) presented a novel lattice Boltzmann scheme to 158 simulate viscoelastic fluid flows, and stated that LBM results were found to be in good 159 agreement with analytical and other numerical results. In this sense, some works were 160 performed earlier by (Degruyter et al., 2010) combining LBM and X-ray µ-CT for the 161 calculation of permeability of volcanic pumices. (Kadauw, 2014) characterized the local 162 density of sand mold using industrial computed tomography, and found good agreement with 163 the experimental density of sand mold. Some typical results were reported recently by 164

165 (Sivarupan et al., 2018) for the use of X-ray  $\mu$ -CT to characterize the additively processed 166 porous structure like 3DP sand mold. (Anbar et al., 2019) used LBM to predict permeability 167 from a computer-generated sphere packing, and to study the impact of sand compaction from 168 the simulations. However, no other literature review exists tackling the particular case of 169 permeability characterization of 3DP sand molds from  $\mu$ -CT digital images using LBM and 170 PNM.

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The current work will describe an accurate and rigorous method to characterize the physical 172 properties of such additively processed sand mold from the digital images provided by X-ray 173 174  $\mu$ -CT. The first point of inquiry is, what is the real local permeability of 3D printed structure? To achieve that goal, a set of X-ray µ-CT experiments are first performed on additively 175 processed silica samples with different silica grain sizes and binder percentage. The 176 microstructural properties are secondly determined through the use of image analysis 177 techniques and PNM. Then, LBM numerical simulations and analytical methods are used to 178 predict the permeability of the samples, and the results are subsequently compared to 179 experimental measurements provided by traditional techniques. 180

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#### 182 **2.** Materials and methods

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#### 184 2.1. Manufacturing process of 3DP sand mold specimen

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186 The raw materials in the current experiments were silica sand and a furfuryl-alcohol-187 composed binder (furan resin binder) with a density of (1.1-1.2) g/cm<sup>3</sup>, as provided by 188 (ExOne, 2014). The silica sand particles used in the present experiments had a mean particle
189 diameter of 140 µm and 190 µm as specified by the supplier in (ExOne, 2013).

190

The samples were designed with NetFabb<sup>TM</sup> software and subsequently converted to .stl 191 format. The designed samples were printed with an ExOne S-Print-Furan 3D printing 192 machine, over a job-box size of  $800 \times 500 \times 400 \text{ mm}^3$ . The process of 3D printing began by 193 adding sulfonic acid (0.18 wt% of the sand) with 8 kg of sand inside a mixing chamber. The 194 acid-activated sand mixture was then transferred to the re-coater. Successive layers of sand 195 grains were added and compacted over the build platform by means of a re-coater head. 196 197 Furfuryl alcohol binder was then gradually injected by the print head nozzle on top of these compacted sand layer beds in order to bind them. The injected furan-resin-binder droplets 198 tend to form a coating layer over individual sand grains. This causes the resin-bonded sand 199 200 grains to crosslink with each other by forming a resin bridge between the sand grains. The additive processing of resin-bonded sand in layers continued until the designed part is 201 fabricated. This resin bridge in between the sand particles hardens gradually, hence providing 202 strength to the printed mold. 203

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For the X-ray CT analysis, 10 small-grain and 10 big-grain cylindrical samples with different binder percentages were printed and named accordingly as provided in Table 1. A set of 20 (5  $\times$  2 different binder content  $\times$  2 different grain size) cylindrical specimens were printed for the experimental permeability measurements, with a diameter of 50 mm and height of 50 mm.

Sample	Binder content (wt%)	Average grain size (µm)
Small Grains with High Binder content (SGHB)	~2	140
Small Grains with Low Binder content (SGLB)	~1	140
Big Grains with High Binder content (BGHB)	~2	190
Big Grains with Low Binder content (BGLB)	~1	190

#### **Table 1.** 3DP specimens used for analysis

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The choice of the binder percentages was based on the recommended values for binder 214 contents (0.9% - 2%) reported in previous research by (Hawaldar and Zhang, 2018). The 215 dimensions of the 3D printed parts for X-ray µ-CT tests were measured manually using 216 Vernier caliper, with top height of  $12 \pm 0.02$  mm, base height of  $10 \pm 0.02$  mm, top diameter 217 of  $4 \pm 0.02$  mm and base diameter of  $6 \pm 0.02$  mm, respectively (the uncertainty corresponds 218 to 95% confidence interval), Fig. 2(d). The temperature of the 3D printing room was 219 controlled at 25  $\pm$  2 °C and the measured relative humidity of the room was 40  $\pm$  10%. A 220 detailed experimental investigation of the effects of mass transport improvement on 221 mechanical strength of 3DP sand mold was presented in previous works by (Mitra et al., 222 2018), (Mitra et al., 2019) and (Ramezani Dana and El Mansori, 2019). 223

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225 2.2. Volumetric reconstruction of 3DP mold via X-ray tomography

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227 2.2.1. X-ray micro computed tomography: image acquisition and post-processing
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In the present study, reconstructed 3D tomographic images of 3DP specimens were used to 229 extract information on microstructural characteristics (grains, pores, porosity, tortuosity) and 230 permeability through image analysis, PNM and LBM simulations. The X-ray µ-CT images 231 were obtained at a facility of CEA LIST (NDT department). The X-ray equipment consists of 232 a micro-focus X-ray generator, a flat panel detector, and a turn-table, situated in a large 233 inspection cell which enables the addition of instrumentation for in-situ characterizations. The 234 X-ray generator is a Viscom 225 kV (320 W) model with a micro-focus spot-size. The 235 detector is a Perkin Elmer XRD0822 model having 1024 x 1024 pixels of 200x200 µm<sup>2</sup> in 236 size, and the acquisitions were performed in a classical setup with a rotating sample (360°) 237 and static source and detector positions. The optimum scan settings for the specimens were 238 determined, obtaining 100 kVp, 60 µA, and 1 second exposure time. For each CT scan, a 239 number of 900 projections were acquired, with an integration time of 1 second. The total 240 acquisition scan was about 30 minutes. The scan facility uses a temperature controlled 241 inspection cell and therefore the impact of temperature variations is considered negligible. 242 The magnification factor was set to 40, which gives a voxel size of 5  $\mu$ m<sup>3</sup> in the CT images. 243 The reconstructions and preliminary analysis were performed by using VGSTUDIO MAX<sup>TM</sup> 244 commercial software at a facility of CEA LIST (NDT department). The setup is shown in Fig. 245 2 as well as the sample holder and the details of specimens. 246



Fig. 2. Different views and schemes of the experimental X-ray  $\mu$ -CT setup showing: (a) the robotic X-ray inspection platform, (b) a schematic design of the sample holder (c) the sample holder and (d) a zoom-in view including the dimensions of the sample.

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For the morphological assessment of 3DP sand mold, the acquired 3D images were binarized and analyzed using the default algorithms provided by (Schindelin et al., 2012) included in ImageJ and subsequently post-treated using different software: ParaView by (Ayachit Utkarsh, 2015), PALABOS by (Latt J, 2009) and OPENPNM by (Gostick et al., 2016). The post-treatment procedure starts by cropping and scaling the raw stack of images, resulting in the cross-sectional dimensions displayed in Fig. 3. Reconstructed X-ray  $\mu$ -CT images were then filtered using a variance weighted mean filter to reduce the effect of background noise. A

median filter of 2 voxels was applied, as shown in Fig. 3(b), to reduce noise without merging 259 the solid particles. The cropped image was then binarized using the Otsu algorithm by (Smith 260 et al., 2010) and was converted into an 8-bit greyscale thresholded image, as shown in Fig. 261 3(c). The reconstructed pixel data were then converted into an 8-bit grayscale image. It should 262 be noted that a 3DP specimen consists of three phases with different attenuation coefficients: 263 silica sand, resin binder and air (pores). It is to be noted that the binder produces a low 264 contrast with respect to silica and is difficult to isolate in a CT image. Therefore, only two 265 phases, e.g. void and solid, were identified in the present experiments. However, the absence 266 of binder in the segmented image is not expected to significantly alter the computed 267 permeability values, due to the low binder contents (1 - 2 wt%) and based on previous results 268 as shown by (Mitra et al., 2019). Furthermore, the thresholding of the CT data was carried out 269 in an iterative manner and validation of the threshold was performed through comparison of 270 the estimated porosity to the porosity measured with a classical mass weighting apparatus. 271

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Fig. 3. Steps during post-treatment of the acquired images: (a) raw image (2D slice), (b)
median filter treatment and (c) converted to 8-bit greyscale binary image. White represents
interstices and black corresponds to solid grains in the binary image.

The sand grain shape and size plays an important role in the fabrication of 3DP sand mold, as 280 they deeply impact the permeability of the sand molds, hence casting quality. The finer the 281 282 silica grains, lower the permeability will be, similarly the coarse silica grains will lead to a higher permeability. Grains are generally categorized based on their shapes; rounded, sub-283 angular and angular. Rounded grains lead to high permeability of sand mold, due to least 284 contact with other grains during the sand compaction. However, these kinds of grain shape do 285 not pack up to its maximum, hence lacks strength. Whereas sub-angular grains have low 286 permeability with high strength values compared to the rounded grains. The angular grain 287 provides higher strength to the 3DP mold, but with low permeability due to tight packing of 288 grains. Therefore it was of great importance to characterize the grain size distribution along 289 with their forms, as it directly affects the casting quality. 290

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For the analysis of the silica grains size distribution, Morpholib - Distance Transform 292 Watershed 3D algorithm by (Legland et al., 2016) included in ImageJ was applied to the 293 thresholded images in order to separate touching objects (creating a border far from the center 294 295 of the overlapping object). The watershed segmentation algorithm detects and separates pore bodies in 2D or 3D images. Then, the connected components are scrutinized using Analysis 296 3D – Labelling plugin by (Boulos et al., 2013) from ImageJ. By using this algorithm, a new 297 volume was generated in which all the particles were labeled. From the generated results, the 298 299 equivalent diameter of each silica grain  $d_g$  was calculated using Eq. 1:

$$d_g = \sqrt[3]{6 \times \text{volmarch}/\pi}$$
(1)

with *volmarch* being the volume in marching cubes. Then, a result file in .xl format was
generated by using the Analysis 3D – Parameter plugin by (Boulos et al., 2013) listing several
parameters: volume in pixel, volume in marching cubes, surface with marching cubes. A
Granulometry-histogram plot was plotted using the total number of labeled particles as a
function of particle diameter as obtained from Eq. 1. Then, the sphericity of the particles was
computed using the following formula (nearly-spherical shapes approaching value 1):

307

sphericity = 
$$6 \times \text{volmarch} \times \sqrt{\pi/\text{surfacemarch}^3}$$

308

Where *surfacemarch* is the surface with marching cubes as shown by (Boulos et al., 2013).
Furthermore, the porosity of the 3DP specimen was calculated by dividing summation of
resulting *volmarch* values by the size of the reconstructed image multiplied by total number
of slices. Also, standard Kozeny–Carman equation (bundle of cylindrical capillaries model)
was used to calculate permeability k from the obtained average grain diameter and pore space
volume from the characterized µ-CT images by:

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$$\kappa = \frac{\varepsilon_{bed}^3 d_s^2}{180(1 - \varepsilon_{bed})^2} \tag{3}$$

(2)

316

where  $\varepsilon_{bed}$  is the average porosity of the  $\mu$ -CT images of the 3DP specimen and  $d_s$  is the average diameter of the silica grains.

To go further, the pore connectivity Z and the geometric tortuosity  $\tau$  of the 3D printed sand 320 mold specimens was also computed through an iterative-thinning algorithm (Median axis 321 algorithm) by using Skeletonize 3D and Analyze Skeleton plugins from ImageJ by (Ignacio 322 Arganda-Carreras et al., 2010) for all the 3DP specimens (SGLB, SGHB, BGLB, and BGHB). 323 The number of branches that originate from a junction (3, 4 and >4 branches) is termed as 324 pore connectivity, and the ratio between the regular and the Euclidean length of such branches 325 is termed as geometric tortuosity. A result window from the plugin displays the node-to-node 326 distances  $(d_i)$ , Euclidian distances  $(d_{euclid})$ , total number of junctions  $(n_i)$ , total number of 327 triple-branch junctions  $(n_t)$ , total number of quadruple-branch junctions  $(n_q)$ . Any junctions 328 above that is a high-order junctions  $(n_x)$ . It was shown earlier by (Hormann et al., 2016), that 329 the pore connectivity (Z) can be calculated from  $(n_i)$ ,  $(n_t)$ ,  $(n_a)$ , and  $(n_x)$ , using Eq. 4 and 330 Eq. 5: 331

$$Z = 3\frac{n_t}{n_j} + 4\frac{n_q}{n_j} + 5\frac{n_x}{n_j}$$
(4)

$$\frac{n_x}{n_j} = 1 - \frac{n_t}{n_j} - \frac{n_q}{n_j} \tag{5}$$

Where,  $n_t/n_j$ ,  $n_q/n_j$ , and  $n_x/n_j$  provides the fraction of nodes connecting 3, 4 and >4 branches respectively.

And the tortuosity was calculated as being the average ratio between node-to-node network distances ( $d_i$ ) and Euclidean distances ( $d_{euclid}$ ) as shown by (Ignacio Arganda-Carreras et al., 2010) and (Hormann et al., 2016):

$$\tau = \frac{1}{n} \sum_{i=1}^{n} \frac{d_i}{d_{euclid}} \tag{6}$$

The results in terms of pore connectivity (Z) and tortuosity ( $\tau$ ) are provided in Table 2. It can 338 be observed that most junctions have 3 branches, a significant number of junctions have 4 339 branches and only a few present 5 or more branches. An average pore connectivity value of Z 340  $\approx$  3 is obtained. In this regard, (Sivarupan et al., 2018) showed in a previous work that the 341 speed at which the recoater spreads the sand particles on the job box platform affects the pore-342 connectivity, hence affecting the permeability. It can be deduced from the results displayed in 343 Table 2 that the size of the grain does not affect pore connectivity, in contrast to the case of 344 recoating speed. 345

Sample	n <sub>t</sub> /n <sub>j</sub>	n <sub>q</sub> /n <sub>j</sub>	n <sub>x</sub> /n <sub>j</sub>	Pore connectivity (Z)	Tortuosity (τ)
SGHB	0.721	0.211	0.067	3.346	1.223
SGLB	0.703	0.243	0.052	3.348	1.221
BGHB	0.833	0.131	0.034	3.201	1.218
BGLB	0.773	0.176	0.049	3.275	1.225

**Table 2.** Results from median axis algorithm, showing the pore connectivity and tortuosity

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## 348 2.3. Computational simulation of fluid flow in 3DP sand mold using Lattice Boltzmann 349 Method

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A volume of  $367 \times 367 \times 367$  voxel (corresponding to  $1835 \times 1835 \times 1835 \ \mu\text{m}^3$ ) was cropped from the original reconstructed image with voxels of  $5^3 \ \mu\text{m}^3$ . The cropped image was then binarized using the procedure presented in subsection 2.2.1. The porosity was then computed by dividing the number of pore space voxels (white) by the total volume of the image stack.

The volume of the image being used as input to numerical simulations must be large enough 356 to produce a representative and statistically meaningful value of permeability for the 3DP 357 sand mold. While too big volumes would require a powerful and parallel computer clusters, 358 the Representative Volume Element (RVE) must lead to statistically meaningful results while 359 reducing computation time. Therefore, four different sizes of representative were selected 360 from the original cropped binary image: 200×200×200 voxel, 150×150×150 voxels 361 100×100×100 voxels and 50×50×50 voxels, as shown in Fig. 4, corresponding to 362 1000×1000×1000 µm<sup>3</sup>, 750×750×750 µm<sup>3</sup>, 500×500×500 µm<sup>3</sup>, and 250×250×250 µm<sup>3</sup> 363 volumes, respectively. These 4 cropped segmented stacks were then used as inputs to the 364 LBM numerical simulations performed with Lattice-Boltzmann Method (LBM) solver 365 PALABOS in order to determine the RVE for permeability calculation. The entire process 366 was repeated for all the binder content-grain size combinations listed in Table 1. 367





Fig. 4. Images of different dimensions used to determine the Representative Volume Element
(RVE) of the BGLB specimen. Pores are displayed in white and silica sand grains in black on
the binary image.

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The numerical simulations were performed by using the open-source Lattice-Boltzmann 374 Method (LBM) solver PALABOS (Parallel Lattice Boltzmann Solver). LBM is highly 375 reliable and has been applied extensively as discussed by (Chopard B et al., 2002). (Heijs and 376 Lowe, 1995) used LBM to predict the permeability of a random array of spheres and clay soil, 377 and found that the predicted permeability is consistent with the experimentally measured 378 values. (Ferrol and Rothman, 1995) studied the numerical simulations of mass transport 379 through 3D tomographic images of Fontainebleau sandstone, and found that the LBM 380 simulations were similar as compared to the finite difference calculations and with the 381 laboratory experimental measurements. It was studied and verified earlier by (Auzerais et al., 382 1996) that X-ray micro computed tomography (µ-CT) along with LBM can be used for 383 modeling the fluid flow phenomena through complex porous geometries to study the 384 permeability. (Degruyter et al., 2010) combined X-ray µ-CT and LBM solver PALABOS to 385 perform numerical simulations of gas flow through volcanic pumices, and validated the 386 method by comparing the resulting data with the experimentally obtained values. Hence for 387 the present numerical simulation, LBM was used to predict the permeability of the additively 388 processed sand mold. 389

390

For the numerical simulation of mass transport through the 3D tomographic image of 3DP specimen, a bounce-back boundary condition (no-slip boundary condition) was applied in between the interfaces of pore space and silica sand grains. In PALABOS-LBM numerical

simulation, a D3Q19 lattice scheme is proposed as demonstrated earlier by (Hecht and 394 Harting, 2008). D3Q19 lattice describes the fluid flow in three dimensions with 19 possible 395 velocity vector directions, along with the zero velocity as shown by (Hecht and Harting, 396 397 2008) and (Ding and Xu, 2018). A standard Bhatnagar Gross-Krook (BGK) collision operator was applied to the D3Q19 lattice scheme. A constant pressure gradient ( $\nabla P$ ) was applied 398 through the porous medium, and the initial velocity within the interstices was set to zero. The 399 imposed values of  $\nabla P$  were low enough to ensure creeping flow regime (Darcy flow). Non-400 slip boundary conditions were applied and the lateral boundaries of the porous geometry 401 shown in Fig. 5. Permeability (k) was then measured on the non-dimensional lattice unit 402 system from the obtained pressure and velocity maps using Darcy's equation: 403

404

$$-\frac{dP}{dz} = \frac{\mu}{k}v$$
(7)

405

where dP/dz is the pressure gradient along the main flow z-direction,  $\mu$  is the dynamic viscosity, v is Darcy velocity and k is the permeability of the 3DP mold. The calculation methodology used by PALABOS to measure the permeability of porous media involves in solving a modified version of the actual Darcy's equation. Here, *Q/A* is denoted by the term v, which is the mean fluid velocity through the porous media or as stated earlier as Darcy's velocity. Q is the flow rate of fluid through a sample of cross section area A.



Fig. 5. Boundary conditions for numerical simulation

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For the numerical simulation, the binary image was converted into a .DAT-file as needed by 416 417 PALABOS software to be able to read the entire porous 3D printed sand mold geometry (along with labeled pores and grains), Fig 6. The DAT-file conversion procedure along with 418 the code for MATLAB was used from the tutorial as provided in the PALABOS website by 419 (Degruyter et al., 2010). The code allows for the separation between grains and pores, by 420 creating an interfacial boundary, as shown in Fig. 6(b). Then a constant pressure was imposed 421 422 at the inlet of the geometry. The bounce-back boundary condition was applied to the interface. Fig. 6(c). shows an example of simulated velocity distribution over a 2D cross-section of an 423 X-ray  $\mu$ -CT image. k was first obtained in non-dimensional lattice units and was then 424 425 converted to SI units by considering the squared resolution of the original µ-CT image.



Fig. 6. Visualization of steps in conversion of a μ-CT image for velocity distribution simulation in the case of the SGHB specimen (200 voxels): (a) 2D slice of the binary volume and (b) converted image for simulation with pore space (dark blue pixel), grains (yellow pixel) and grain boundary interface (light blue pixel) where the bounce-back boundary condition is implemented. (c) Simulated velocity distribution through a cross-section.

434 2.4. Pore network extraction from micro-CT images: pore and throat size distributions

435

A PNM approach was followed in order to characterize the dimensions of the pore bodies and 436 constrictions of the 3DP molds, by using the images displayed in Fig. 7 as inputs. In the 437 438 present work, the pores and the throat networks were then extracted from the obtained X-ray  $\mu$ -CT of the 3DP specimens using the SNOW and GETNET algorithm as shown by (Gostick, 439 2017). This algorithm was previously implemented on various porous medium ranging from 440 fibrous mats to sandstone, for the extraction of pore and throat sizes, and predicting 441 permeability values. The open-source algorithm called as SubNetwork of the Oversegmented 442 Watershed (SNOW) as provided by (Gostick, 2017) was utilized in the current investigation 443 the extract the pore-network from the X-ray µ-CT images. The extracted pore and throat 444

diameters correspond to the diameter of the largest spheres that can be inscribed in a porebody and a constriction, respectively.

447

The method for pore network extraction starts by using GETNET.py code as provided by 448 (Gostick, 2017), which extracts a conventional pore network from the provided µ-CT image 449 of voxel size  $200^3$ . As stated by (Gostick, 2017) the code works in 4 steps, first it extracts the 450 distance map of the pore space (distance transform), secondly a filter was used on the distance 451 map to smoothen the image and to remove the saddles and the plateaus, thirdly merging the 452 peaks that are too close to each other and then lastly assigning the pore space voxel to the 453 appropriate pores using a marker-based watershed algorithm. Recently, (Rodríguez de Castro 454 455 and Agnaou, 2019) have used the code to extract the pore and throat network of a sandy porous structure. Similarly, for the present extraction, the X-ray µ-CT image of 3DP specimen 456 was first thresholded and then converted into an 8-bit file. Then, using the SNOW algorithm 457 in PYTHON, the X-ray µ-CT image is imported for further characterization. This import class 458 then extracts all the information of the provided µ-CT image, such as pore and throat sizes, 459 their locations and their network connectivity. All pore and throat properties are stored in 460 Numpy arrays, which can be easily accessible at later stage for generating the network. 461



464 Fig 7. X-ray μ-CT image for all specimens used for PNM, (a) SGLB, (b) SGHB, (c) BGLB
465 and (d) BGHB

Permeability is strongly related to the dimension of the pore constrictions (throats), as most 466 pressure loss is generated in these regions. (Bonnet et al., 2008) studied in detail the effect of 467 form, shape, or structure on flow law properties in metallic foams. On the other hand, 468 (Degruyter et al., 2009) and (Degruyter et al., 2010) showed that the tortuosity ( $\tau$ ), porosity ( $\varepsilon$ ) 469 can be directly correlated according to Archie's law ( $\tau^2 = \varepsilon^{-m}$ ). (Huang et al., 2015) also 470 studied the flow properties within a digital image of fibrous porous medium to predict the 471 permeability and validated the described model. (Degruyter et al., 2009) and (Degruyter et al., 472 2010) also developed a model to calculate k directly from the characteristic diameter of the 473 474 throats ( $d_{throat}$ ) and Archie's law:

$$k = \frac{\varepsilon^{\rm m} d_{\rm throat}^2}{32}$$

(8)

476

The permeability was then calculated by using the average throat size provided by thenetwork model.

479

#### 480 2.5. Experimental approach: Local porosity and permeability

481

A detailed review of experimental characterization for density, porosity and permeability 482 method was published recently by (Mitra et al., 2018) and (Mitra et al., 2019), so this section 483 contains only a short description of the method. The weight of the 3D printed specimens was 484 measured using a laboratory precision balance and the density of printed sample was 485 measured as mass divided by volume. The experimentally measured density of 3D printed 486 sand mold was ~1.3 g/cm<sup>3</sup>. The particle density is the density of silica sand with ~2.6 g/cm<sup>3</sup>. 487 From the measured density of 3DP specimen and silica sand density, the porosity of the 3D 488 printed samples was measured as, 489

490

$$Porosity (\%) = 1 - \frac{Density_{bulk}}{Density_{silica}}$$
(9)

491

The porosity values measured from experiments were close to 49-51% for all printed specimens, with a standard deviation of 0.25%. Also, the permeability of the 3DP sand mold samples was determined with a permeameter device (Simpson-Electrical), following the recommendations of the American Foundry Society (AFS) and the same procedure presented in previous works by (Coniglio et al., 2017), (Sivarupan et al., 2017), (Mitra et al., 2018) and (Mitra et al., 2019). Therefore the entire procedure for the permeability experiment will not be presented here. The initial dimensions of the 3D printed parts (cylinders) for experimental gas permeability characterization were of  $49.8 \pm 0.01$  mm in length and of  $49.9 \pm 0.02$  mm in diameter. The relationship for the measurement for gas permeability (GP) is expressed by the following equation:

502

$$GP = \frac{V \times h}{F \times p \times t}$$

(10)

503

Where V denotes the air volume, h denotes the length of the cylindrical 3DP specimen, F denotes the cross-sectional area of the 3DP specimen, p denotes the pressure and t denotes the passage time for volume of air in minutes. An average permeability value of  $5.57 \times 10^{-11}$  m<sup>2</sup> or ~56.43 Darcy was measured for the small grain (SG) specimens, and  $9.02 \times 10^{-11}$  m<sup>2</sup> or ~91.39 Darcy for the big grain (BG) specimens.

509

#### 510 **3. Results and discussion**

511

#### 512 3.1. Grain size distribution and sphericity of silica particles

513

It is to be noted that since the binder was associated to the solid phase in the CT images, an individual effect of the binder cannot be assessed and therefore the values for low binder and high binder were merged together for the assessment, Fig. 8. The procedure presented in

subsection 2.2.2 was applied to all the segmented X-ray µ-CT images in order to obtain the 517 grain size and sphericity distributions of the silica particles. A normal distribution could be 518 observed for the grain size distribution. The extracted silica grain diameter  $d_g$  for small grain 519 specimen varied from ~57  $\mu$ m to ~331  $\mu$ m, with mean d<sub>g</sub> of ~171.98  $\mu$ m and the extracted d<sub>g</sub> 520 for big grain specimen varied from ~61  $\mu$ m to ~409  $\mu$ m, with a mean grain diameter d<sub>a</sub> of 521 ~208.05  $\mu$ m. A more detailed report regarding the granulometry of the 3DP specimens is 522 provided in Table 3, showing the values for high and lower binder contents. GSD has a 523 profound effect on the permeability of the 3DP sand mold. It can be seen that for both small 524 525 and bigger grains, there is a similar narrow distribution of grain sizes, hence provides good permeability for fabricated 3DP sand mold. Because sand grains with wide range has higher 526 compaction leading to high density and low permeability compared to the narrow distribution. 527



529 Fig. 8. Combined (a) grain size distribution for small grains and big grains, and (b) sphericity

530

distribution.

Also, the sphericity measured from the X-ray µ-CT image provides information about the 532 particle shape, which affects grain packing density, hence varying porosity and permeability. 533 We note the fact that grains with different shape might have identical sphericity values. The 534 results in terms of sphericity are listed in Table 3. It is observed that the sphericity values of 535 the bigger grain size specimens were higher than those of the small grain size specimens. 536 Some examples of extracted grains from the big grain specimens are shown in Fig. 9. It can be 537 noticed that the grains are far from being a perfect sphere, with an average sphericity value of 538 ~0.6. As we discussed earlier the shape can be rounded, angular, sub-angular, however in the 539 present case, it can be observed that the grains are mostly sub-angular. All the results of the 540 sphericity of the specimens are shown as a histogram in Fig. 8. 541

542



Fig. 9. (a) Examples of silica grain with different sphericity number in the BG specimen. (b)
SEM image of a 3DP specimen, showing the silica grains.

546

From the obtained granulometry, using the porosity and mean grain diameter, the permeability of the 3DP specimens were predicted with the Kozeny-Carman equation (Eq. 3) as shown in Table 3. It is to be noted that since the binder was associated to the solid phase in the CT images, an individual effect of the binder cannot be assessed and therefore the values

551 for low binder and high binder are very close.

552

553

Tal	ble 3	<b>3.</b> F	Result	ts i	from	image	anal	lysi	IS
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Sample	Mean $d_g$ (µm)	Mean	Mean porosity	Permeability	Permeability
Туре		Sphericity	(%)	(m <sup>2</sup> )	(Darcy)
SGLB	154.07	0.56	50.97	$6.593 \times 10^{-11}$	66.80
SGHB	156.85	0.55	49.37	$6.182 \times 10^{-11}$	62.63
BGLB	210.11	0.66	48.48	$1.003 \times 10^{-10}$	101.62
BGHB	207.04	0.67	49.35	$1.077 \times 10^{-10}$	109.12

554

#### 555 3.2. Permeability of the printed samples as obtained from LBM numerical simulations

556

The steady-state velocity maps provided by the LBM simulations introduced in subsection 557 2.3., throughout the simulated specimens were represented using PARAVIEW software as 558 shown in Fig. 10. It can be deduced from this figure that the velocity distribution is not 559 uniform throughout the porous media, as expected due to the varying cross-section 560 dimensions of the interstices. The ratio between pressure difference ( $\Delta P$ ) and the volumetric 561 flow rate was constant for all the tested values of  $\Delta P$ , confirming creeping regime. Different 562 image sizes  $(50^3 \text{ voxel}, 100^3 \text{ voxel}, 150^3 \text{ voxel}, \text{ and } 200^3 \text{ voxel})$  were used in the simulations 563 for the computation of k. Table 4 provides the permeability values for all the specimens as 564 provided by LBM solver PALABOS by using the modified Darcy's equation (Eq. 7) as stated 565 earlier in section 2.3. Indeed, from Fig. 11, it can be observed that the permeability value for 566

567 50 voxel image is lower than that of 100 voxel, 150 voxel and 200 voxel image stack for all 568 the 3DP specimens. The permeability values approached a plateau value when the size of the 569 RVE was greater than 100 voxels. Therefore, it is suggested to use an input volume of 500 570  $\mu$ m<sup>3</sup>, which corresponds to the size of 3 equivalent layers (3×190  $\mu$ m or 3×140  $\mu$ m) of silica 571 grains for 3DP specimens with average grain diameter of 140  $\mu$ m and 190  $\mu$ m. Bigger image 572 sizes would lead to higher simulation times without any significant improvement in accuracy.



Fig. 10. Velocity map in lattice units through specimens of, (a) 50, (b) 100, (c) 150, and (d)
200 voxel. (Warmer colors represent higher velocity)

Image Size	Porosity	Permeability	Permeability
(voxel)	(%)	( <b>m</b> <sup>2</sup> )	(Darcy)
	Small Gr	ain Low Binder (SGLB	)
50	51	$4.431 \times 10^{-11}$	44.89
100	50	$4.844 \times 10^{-11}$	49.08
150	51	$5.215 \times 10^{-11}$	52.84
200	52	$4.842 \times 10^{-11}$	49.06
	Small Gro	ain High Binder (SGHE	3)
50	49	$4.403 \times 10^{-11}$	44.61
100	51	$5.475  imes 10^{-11}$	55.47
150	50	$5.077 \times 10^{-11}$	51.44
200	53	$5.166 \times 10^{-11}$	52.34
	Big Gra	in Low Binder (BGLB)	
50	49	$3.889  imes 10^{-11}$	39.41
100	51	$8.801 \times 10^{-11}$	89.17
150	49	$8.788  imes 10^{-11}$	89.04
200	52	$9.092 \times 10^{-11}$	92.12
	Big Grau	in High Binder (BGHB)	)
50	49	$4.171 \times 10^{-11}$	42.26
100	52	$9.157 \times 10^{-11}$	92.78
150	53	$9.027 \times 10^{-11}$	91.46
200	53	$9.189  imes 10^{-11}$	93.11



Fig. 11. Effect of input geometry volume on the computed value of permeability

582

The computed results of permeability for 3DP specimen through PALABOS with different 584 grain and binder percent samples can be compared with the predicted analytical results and 585 586 image analysis results. The agreement is good between the analytical method, the image analysis and the experimental results for all the 3DP specimens (SGLB, SGHB, BGLB, and 587 588 BGHB). The permeability calculations obtained with PALABOS are in good co-relation with 589 the experimental measurements performed with the 3DP specimen, as shown in Table 4. Although it is of worth mentioning that an analytical permeability value of  $4.9 \times 10^{-11}$  m<sup>2</sup> (or) 590 ~49 Darcy was calculated with Kozeny-Carmen equation (Eq 3), by using the average grain 591 size of 140 micron (as provided by the ExOne sand provider) and measured porosity of 49.2 592

%. And also a permeability of  $9.071 \times 10^{-11}$  m<sup>2</sup> (or) ~91 Darcy was calculated) with the 593 average grain size of 190 micron (as provided by the ExOne sand provider) and measured 594 porosity of 49.5 %. A deviation of permeability could be observed compared to analytical 595 permeability value as the prediction of Kozeny-Carmen is based on the particles being a 596 perfect sphere (the equation uses the mean diameter, ds), whereas in the present scenario the 597 particle is close to being a perfect sphere (average sphericity = 0.65). The analytically 598 predicted permeability value using Kozeny-Carmen equation worked as a reference for the 599 600 permeability measurements. It can be observed from the table that, it is possible to predict the absolute permeability of 3DP sand mold using the non-destructive LBM simulation and is a 601 602 very strong method for mass flow simulation in complex 3D printed sand mold.

603

# 3.3. Pores and Throats Size Distributions of the 3D printed samples as provided by pore network modeling

606

607 PNM provides a reasonable prediction of mass transport properties at pore scale and offers the flexibility of characterizing macroscopic properties relationship of 3DP sand mold with pore 608 609 structure. With PNM, the complex pore structure of a 3DP sand mold can be represented by a 610 network of pores (pore spaces) and connected throats (narrow paths that connect pores) with simplified geometries. A pore network modeling aims at better representation of pore and 611 throat interconnectivity in a porous medium like 3DP sand mold. All the pore network 612 extractions for different specimens (SGLB, SGHB, BGLB, BGHB) were performed over a µ-613 CT image size of  $200^3$  voxel with a resolution of 5  $\mu$ m per voxel, and are represented in Fig. 614 12. 615



Fig. 12. Extracted pore network for (a) SGLB, (b) SGHB, (c) BGLB and (d) BGHB
specimens.

The pore-size distributions (PSDs) in terms of pore diameter were extracted from the generated pore network and are represented as a histogram, Fig. 13. The extracted pore diameter for SGLB specimen varied from ~19  $\mu$ m to ~226  $\mu$ m, with a mean pore diameter of ~105.84  $\mu$ m and the extracted pore diameter for SGHB specimen varied from ~14  $\mu$ m to ~220  $\mu$ m, with a mean pore diameter of 108.05  $\mu$ m. Similarly, the extracted pore diameter for BGLB specimen varied from ~16  $\mu$ m to ~350  $\mu$ m, with a mean pore diameter of 108.07  $\mu$ m and the extracted pore diameter for BGHB specimen varied from ~18  $\mu$ m to ~320  $\mu$ m, with a

mean pore diameter of ~108.31 µm. Although previous work by (Glover and Walker, 2009) 628 showed that the grain size and pore radius are functionally interdependent, it can be observed 629 that the average pore diameters are very similar for all the specimens (both SG and BG) in the 630 631 currently investigated samples. However, careful observation of Fig. 13 shows that the standard deviation of the PSD is considerably higher for the big sand grains samples ( $\pm$  55.9 632  $\mu$ m for BGLB and  $\pm$  56.1  $\mu$ m for BGHB) as compared to the small sand grains samples ( $\pm$ 633 37.3  $\mu$ m for SGLB and  $\pm$  38.7  $\mu$ m for SGHB). Consequently, the size of the biggest pores in 634 the big grain samples is much higher than for the small grain samples, even if the average 635 pore size is close in both cases. This can be also observed in the red-colored pores of Fig. 12 636 (approximately 350 micrometers of big grains and 230 for small grains) and in the PSDs 637 provided in Figure 13. 638



Fig. 13. Combined (high binder +low binder) pore size and throat size distribution for (a) 641 642 small grains and (b) big grains.

The throat-size distributions (TSDs) in diameter were also extracted from the generated throat 644 network and were then represented as a cumulative histogram with the throat diameter, Fig. 645 13. The extracted throat diameter for SGLB specimen varied from ~5 µm to ~140 µm, with a 646 mean throat diameter of 38.66 µm and the extracted throat diameter for SGHB specimen 647 varied from ~5 µm to ~146 µm, with a mean throat diameter of 44.43 µm. Similarly, the 648 extracted throat diameter for BGLB specimen varied from ~5 µm to ~214 µm, with a mean 649 throat diameter of 56.92 µm and the extracted throat diameter for BGHB specimen varied 650 from ~5 µm to ~220 µm, with a mean throat diameter of 58.42 µm. It can be depicted from 651 the distribution that, the peak values for both cases appear to be near low pore sizes, which 652 defines the microstructure complexity. It can also be observed for big grain specimens that the 653 throats and pores overlap with each other, which suggests that there exist some small pores, 654 which are of similar size as that of the throats. Moreover, the distribution of throat size for all 655

the specimens shows a right-skewed distribution, along with a quantitatively great portion of the small size throats (peak throat size smaller than average), which construct minor flow paths.

659

Table 5. Results from pore network modeling

Sample	Mean Pore	Mean Throat	Permeability	Permeability
Туре	Diameter (µm)	Diameter (µm)	( <b>m</b> <sup>2</sup> )	(Darcy)
SGLB	105.84	38.66	$3.138 \times 10^{-11}$	31.79
SGHB	108.05	44.43	$4.144 \times 10^{-11}$	41.98
BGLB	108.07	56.92	$6.915 \times 10^{-11}$	70.06
BGHB	108.31	58.42	$7.165 \times 10^{-11}$	72.59

From the obtained average equivalent throat diameter and tortuosity, permeability was 662 calculated using the equation described in the previous section, Eq. 8, and the results are 663 presented in Table 5. It can be observed from the results that no significant differences in 664 665 terms of permeability (k) were obtained for small grain samples with different binder content along with big grain samples with different binder content, as the furan resin binder was only 666 associated to the solid phase in the µ-CT images. An individual effect of the binder over pore 667 network structure cannot be assessed and therefore the values for pore and throat diameter for 668 samples with low binder and high binder are very close. 669

670

#### 671 **4. Model efficiency**

672

One of the challenges in foundry is the lack of methods for proper non-destructive 673 characterization of the local permeability of the 3DP sand mold. The X-ray µCT technique 674 overcomes this challenge and allows a non-destructive visualization and characterization of 675 internal volume and the external surface of a sand mold. This paper, for the first time, fully 676 characterizes the intrinsic physical parameters of 3DP sand mold including grain structure, 677 porosity, pore connectivity, tortuosity, pore size distribution, throat size distribution and local 678 density. Table. 6 shows the cumulative results of permeability as obtained by different 679 methods (from traditional experiment, from GSD, from LBM and from PNM). The 680 681 permeability value using the GSD method overpredicts the permeability value as obtained with the traditional experiments. Indeed, the permeability value from GSD using Kozeny-682 Carman equation is based on the particles being a perfect sphere (the equation uses the mean 683 684 particle diameter, d<sub>s</sub>), whereas in the present scenario the particle is close to being a perfect

sphere (average sphericity = 0.65). However, the permeability value obtained with GSD using
Kozeny-Carman equation can still be considered as a reference for other models.

687

Moreover, the permeability values yielded by LBM simulations were found to be close to the 688 results provided by traditional tests. Nevertheless, LBM requires much computational power 689 for larger µ-CT images, hence this method can be time consuming. Therefore, it was crucial 690 to identify the optimum RVE not only to predict reliable permeability values but also to 691 reduce simulation times. An alternative approach to predict permeability from pore-network 692 modelling (PNM) is proposed. Pores are the relatively wide portions of the interstices and 693 694 throats are the relatively narrow portions that separate the pore bodies. The pores and throats 695 space of a 3D printed sand mold can be extracted from the segmented 3D µ-CT image. As can be observed from Table 6, significant differences are reported in some cases between the 696 697 results of traditional experiments and PNM, while the agreement is better between traditional tests and GSD and LBM. Nevertheless, as compared to LBM simulations, PNM require less 698 computational power due to the simplifications of the void-space geometry and topology 699 when constructing the pore network model. The computational time needed for the extraction 700 701 of the pore and throat network on a computer with Intel Xeon processor and 16 GB of memory is in the order of minutes, whereas using LBM computation takes hours. This allows 702 the computation of permeability over larger sampling volumes. However, it should be noted 703 that the computational time can be significantly reduced by using a more powerful and 704 705 expensive supercomputer. (Chauveteau et al., 1996) showed that for unconsolidated porous 706 media where pore throats are much smaller than pore bodies, the viscous dissipation can be considered as being localized only in pore throats. This approximation is quite acceptable in 707 708 many cases, since the pore body-to-pore throat radius is generally quite large, varying from 709 values around 3 for random monosized sphere packs, to around 5 for random packs of sharp-

edged grains with a narrow size distribution. However, in the case of the highly-porous 3DP 710 sand molds investigated in the present work, the pore-to-throat size ratios range from ~1.7 to 711  $\sim$ 2.7 (Table 5). Therefore, the PNM-based estimation obtained with Eq. 8, in which viscous 712 713 dissipation is assumed to be localized only in pore throats, is not expected to be highly accurate, but is still useful to provide a lower permeability bound. Hence, PNM approach can 714 be a reasonable alternative to the traditional experimental, LBM and GSD methods as it takes 715 into account of the microstructural features of the 3DP sand mold and can also easily deal 716 717 with any kind of complex geometry.

718

719

#### Table 6. Permeability measured with different methods

Sample	Traditional experiment	GSD	LBM using 100 voxel	PNM
	(Darcy)	(Darcy)	(Darcy)	(Darcy)
SGLB	56.4	66.8	49	31.79
SGHB	58.9	62.6	55.4	41.98
BGLB	91.3	101.6	89.1	70.06
BGHB	93.2	109.1	92.7	72.59

720

Permeability, porosity, tortuosity grain size distribution, pore size distribution, average pore diameter, throat size distribution, and average throat diameter are essential inputs when predicting gas flow in 3DP molds. It is to be noted that complex porous media like 3DP sand mold have anisotropic properties (mechanical and mass transport) due to variation in printing process parameters. For the present study, only the variation of furan resin binder droplet resolution on silica sand powder bed is studied (different binder percentage) along with different silica grain size, as this affects the properties of complex porous resin bonded 3DP

mold with the recoater speed. The present modeling approaches are advantageous on the 728 prediction of the flow permeability of such complex porous structure like 3DP sand mold 729 directly from the from X-Ray µ-CT digital images. This would help the foundry industry to 730 731 accurately measure the mass transport properties as required as an input for numerical simulations (solidification and filling), to study the effect of printing process parameters 732 (printing speed, binder percentage, grain size, etc.) and thermal degradation of furan resin 733 binder during metal casting. Therefore, the present approaches of merging permeability 734 735 measurements on 3DP sand mold specimens with extraction of throat and pore network structure using for X-ray µ-CT helped in exploring and better understanding the pore 736 construction and its pivotal role on mass flow phenomenon. It also helped us in developing 737 and validating reliable models for non-destructive prediction of gas permeability, which are 738 favorable for carrying out precise risk assessments of harmful toxic pollutants produced 739 during metal casting in foundry industry. 740

741

#### 742 **5.** Conclusion

743

Permeability is one of the most important factors affecting the generation of gas defects 744 during metal casting, so it is of major importance to characterize it. In this work, the 745 advantage of the application of X-ray µ-CT (NDT), Pore Network Modelling methods and 746 Lattice Boltzmann Method in exploring the mass transport properties of additively processed 747 silica sand mold was demonstrated. X-ray µ-CT images were used to compute the porosity, 748 pore size, throat size and the permeability of the 3D printed specimens for different binder 749 contents and grain sizes, using analytical and numerical methods. The permeability predicted 750 in the steady-state was compared with experimental and analytical measurements for layered 751

752	silica grain arrangement. A major advantage of using X-ray CT characterization is the no	n-
753	lestructive nature of the tests. The computed permeability can be used as input to numeric	cal
754	simulations of metal casting allowing the prediction of macroscopic defects. The followi	ng
755	scientific and industrial implications are drawn from the present work:	
756		
757	• The permeability values predicted with LBM from X-ray $\mu$ -CT image of 3DP specim	en
758	are in good agreement with the traditional experimental measurements.	
759		
760	• The proposed non-destructive X-ray $\mu$ -CT technique is an effective and reliable	ole
761	alternative to traditional laboratory experiments for permeability characterization	of
762	additively processed sand molds. The good agreement between the analytical mod	el,
763	traditional experimental estimations and the proposed method based on CT data validat	es
764	this approach.	
765		
766	• An RVE of 100×100×100 voxel corresponding to 500×500×500 $\mu$ m <sup>3</sup> is suggested for	a
767	faster and reliable permeability simulation.	
768		
769	• The characterization of the 3D printed specimen was performed by using available ope	en-
770	source software such as ImageJ, Palabos, and OpenPNM and therefore the propos	ed
771	approach may be used in a broad range of academic or research applications.	
772		
773	• The permeability value predicted using pore network modeling can be a reasonab	ole
774	alternative as it takes into account of the microstructural features of the 3DP sand mold.	
775		

The present findings represent a step forward towards improved prediction of mass transport properties of the 3DP sand molds. However, further characterization of permeability of such additively processed sand mold should be performed with varying average grain diameter, to check the convergence of the present model. Also samples printed with other printing process parameters should be studied.

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'	0	+

- **6.** Acknowledgment

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