Fabrication and Modeling of a Novel Class of Porous Media

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During the second year of the research, which is concerned with fabrication a novel class of porous media with a wide variety of potential applications, as well as carrying out extensive and large-scale computer simulations in order to understand their properties, several sets of new results were obtained and published. The list of the potential applications of the proposed fabrication method is broad, due to the precise control that one has over the pore-size distribution and porosity of the porous material that is fabricated. The method makes it possible to know *a priori* the morphology of the fabricated porous material.

In the original research proposal we had proposed a fabrication method called SPONGE – structured porous network generation: a nonporous surface, such as plastic films, metal foils, or a glass is coated by a salt, such as NaCl, suspended in a non-soluble medium, such as an alcohol or ketone. The salt consists of cubic crystals and, therefore, represents a granular porous medium of non-spherical particles with a distribution of particle sizes. A polymeric film, such as polyolefin or polyvinyl chloride (vinyl), is then hot-pressed over the salt layer, which fills the void space between the salt's crystals, and solidifies upon cooling. The salt layer is then washed off by water. The voids created by removing the salt crystals represent the pores of the porous medium. Granular powders other than salt can also be used, provided that it can be washed off by a proper solvent after the polymeric matrix has solidified.

SPONGE has many distinct advantages over practically all the previous methods, which are as follows. (i) Since the porous material is prepared by invading the packing of salt crystals, washing it off is easy, as the crystals are all accessible through their contact with each other. (ii) The pore-size distribution and pore connectivity of the porous sample are controlled by the size distribution of the salt crystals, their shapes, and their packing. The voids that are generated by washing off the salt are the pores through which fluid flow and transport, as well as sorption and reaction occur. Thus, the size distribution of the pores is, in principle, exactly the same as that of the salt crystals, which can be measured before the porous medium is even fabricated. As a result, one has complete information on the pore space morphology. (iii) One can also design any size distribution by selecting the appropriate crystal shapes and size distribution. Thus, for fabricating porous media to purify the used water produced in the oil industry, the particle size will be selected in such a way that it can capture a significant amount of the impurities and particles that are suspended in the water. (iv) The size of the pores may also be varied in a controlled way. If, for example, we add a small amount of a nonvolatile liquid, such as propylene glycol, glycerin, or a water-soluble polymer to the solvent, then, upon drying, the added liquid or water-soluble polymer build capillary bridges in the contact area between the particles and expand the size of the pores. After imbibition by the molten polymer and its solidification, the salt and the nonvolatile liquid, or the water-soluble polymer, are leached out, leaving behind the larger pores. Larger and longer pores may also be created in the pore space, if the solution is mixed with soluble fibers, or rod-like crystals. After the fibers are washed off, they leave behind large pores. (v) Since the salt crystals form a packing of particles in which all the particles are in contact, there can be no isolated porosity in the final porous media. In fact, due to the packing structure otherwise, the packing will not be mechanically stable. Thus, practically all the pore space is accessible, and there is virtually no dead-end porosity either.

We have succeeded in fabricating the first generation of porous materials by SPONGE. A paper reporting on the method and the results has been submitted, and is in the revision stage.

To understand better the properties of the fabricated porous materials, we have also been carrying out extensive and large-scale computer simulation of packing of the particles that are used in the fabrication of the porous media. During the second year of the research our simulations progressed very significantly. We have studied the effect of the structure of the surface of the particles on the fluid flow, deformation and transport properties of the packings. We assumed that the particles' surface can be represented by a rough self-affine surface, and showed that depending on the degree of roughness one can obtain a variety of packing with distinct deformation properties. Examples are shown in Figures 1 and 2.

In addition, in order to better understand fluid flow in the pore space, we assumed, as the experimental data indicated, that the pores are similar to nano-channels or nanotubes that are connected through nanojunctions. Our simulations indicated that one obtains a variety of intriguing flow regimes, not reported previously.

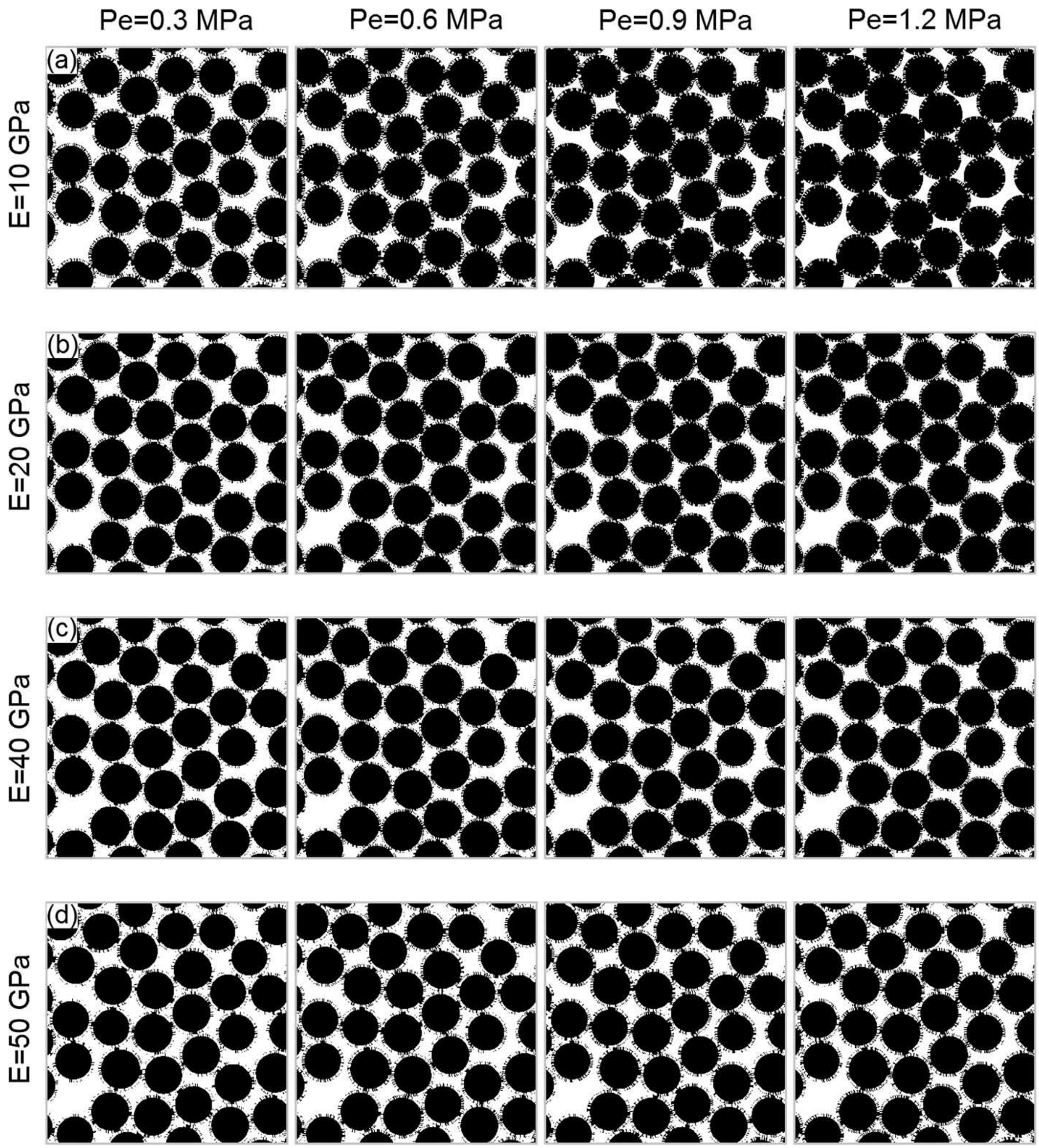
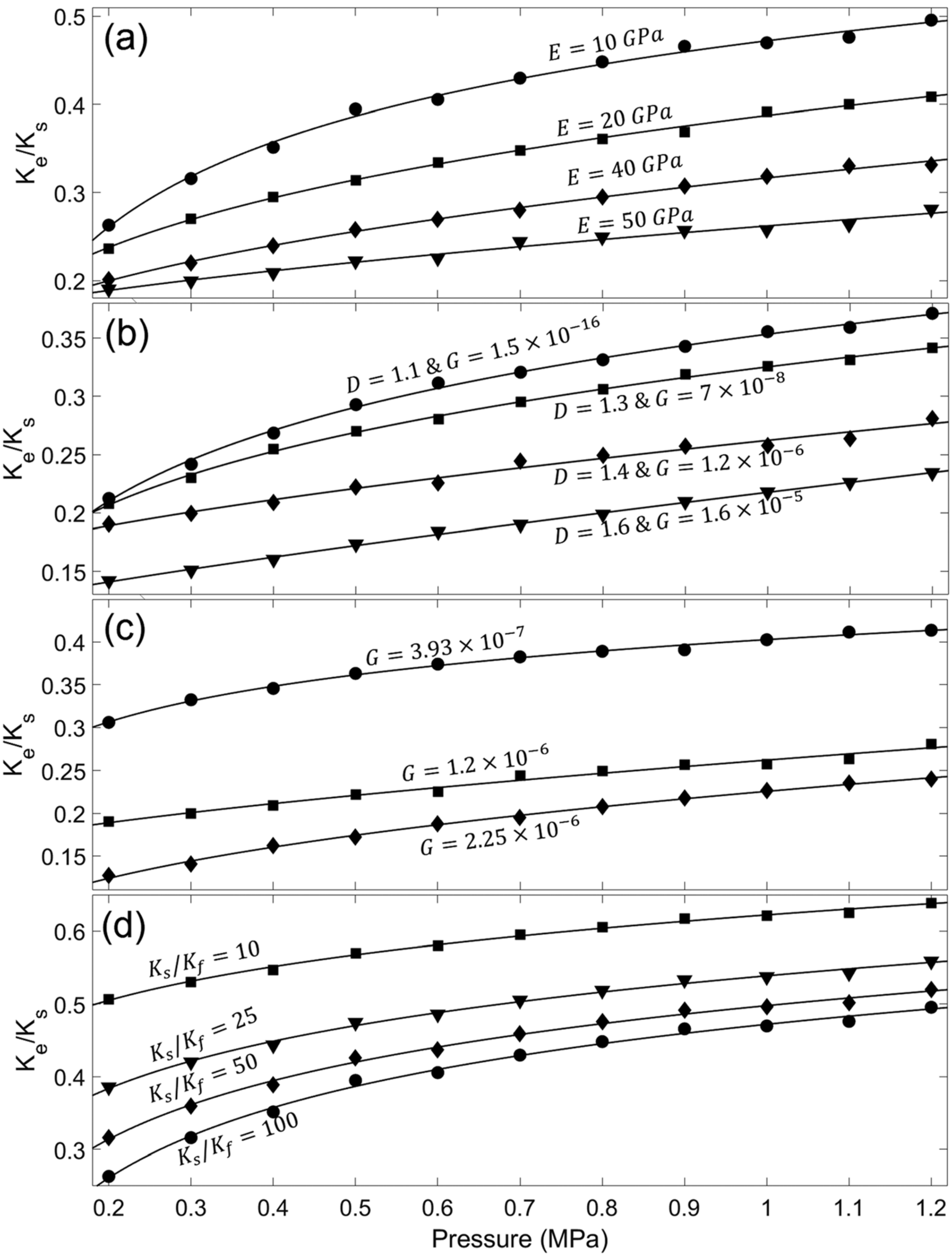


Figure 1: Evolution of the grain contacts of a portion of the packing with the confining pressure P_e and the Young's modulus E.



(a)
E = 10 GPa
E = 20 GPa
E = 40 GPa
E = 50 GPa
(b)
D = 1.1 & G = 1.5 × 10^-16
D = 1.3 & G = 7 × 10^-8
D = 1.4 & G = 1.2 × 10^-6
D = 1.6 & G = 1.6 × 10^-5
(c)
G = 3.93 × 10^-7
G = 1.2 × 10^-6
G = 2.25 × 10^-6
(d)
K_s/K_f = 10
K_s/K_f = 25
K_s/K_f = 50
K_s/K_f = 100
K_e/K_s
Pressure (MPa)
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2

Figure 2: Variations of effective conductivity K_e/K_s with the pressure and (a) the Young's modulus E when the fractal parameters, (D, G) = (1.4, 1.2×10^6), are the same for all the packings; (b) the fractal parameters D and G when the Young's modulus E = 50 GPa is the same for all the packings; (c) G when D = 1.4 and E = 50 GPa, and (d) the ratio of the conductivities of the solid to the fluid (K_s/K_f) when the roughness and elastic parameters are D = 1.4, G = 12×10^7, and E = 10 MPa. Curves are only visual guides and are not calculation results.