Topology, image analysis and wettability

Background and motivation. The flow of multiple fluids – water, oil and gas – in porous materials, such as leaves, lungs, bones and fabrics, as well as soils and rocks, is ubiquitous in nature and manufacturing. To deal with the threat of dangerous climate change, carbon dioxide from burning fossil fuels needs to be safely stored deep underground, in porous rock. The fossil fuels themselves, or at least oil and gas, are themselves recovered from the pore spaces of rock, typically kilometres below the surface. Many engineered materials are made of fibrous fabric: for instance, surgical masks must allow air to flow between the fibres while trapping any droplets of water containing bacteria and viruses.

How the fluids move is controlled by the pore structure itself and the wettability, which measures the relative affinity of water to the solid. For instance, tissues are naturally water-wet and are designed to soak up water: the water is retained within the pore space. On the other hand, waterproof fabrics are water-repellent and do not allow water to enter the pore space. This keeps them dry, while the air-filled porous fabric acts as an insulating layer. There is, however, another feature of porous media which is desirable in many cases, including hydrocarbon recovery and porous layers in fuel cells: how to facilitate the flow of two phases over a wide saturation range where neither phases is retained or trapped in the pore space. Here we have recently shown that the ideal condition is a so-called mixed-wet state where there is a mix of hydrophilic (water-wet) and hydrophobic (water-repellent) surfaces.

The pore-scale imaging and modelling group at Imperial College has pioneered techniques to use X-rays to image porous materials in three-dimensions at micron (thousandth of a millimetre) and sub-micron resolution. They have developed micro-fluidics techniques to study the flow of multiple fluid phases through the pore space, to quantify wettability, and to relate wettability and pore structure to flow and trapping. They have also written bespoke numerical models to predict the flow behaviour.

Recent theoretical developments have shown that multiphase flow in porous media, the role of wettability, and its implications for flow and trapping, can all be understood in terms of principles in topology. This opens up a novel and particularly rich research direction – can we use the information from pore-space images combined with ideas in topology to quantify wettability and then understand and design optimal conditions for either flow or trapping?

Research plan and idea. We start with some basic concepts in geometry. As shown in Figure 1, the sum of the exterior angles of a polygon is 2π, even if – for a concave shape – some of the angles can be negative. If instead we have a shape with a smooth boundary, the integral of the curvature, κ, is 2π. In general, if we have a shape with both smooth regions and angles, the sum of the exterior angles α plus the integral of the curvature is 2π:

$$\sum \alpha_i + \int \kappa \, dl = 2\pi \qquad (1)$$

The same concept can be extended to three dimensions using the Gauss-Bonnet theorem. A smooth two-dimensional surface has two principal curvatures in orthogonal directions. The Gaussian curvature, G, is the product of these two curvatures. The integral of the Gaussian curvature over a shape that is topologically a sphere (that is can be distorted to make a sphere) is 4π. This is a remarkable theorem, as it applies to any shape, however much it is transformed.

How does this relate to flow in porous media? Figure 2 shows a schematic of one phase (say oil or carbon dioxide) on a solid surface surrounded by another phase (water). This is at the small scale within a porous material, so the droplet may be less than 1 mm across.

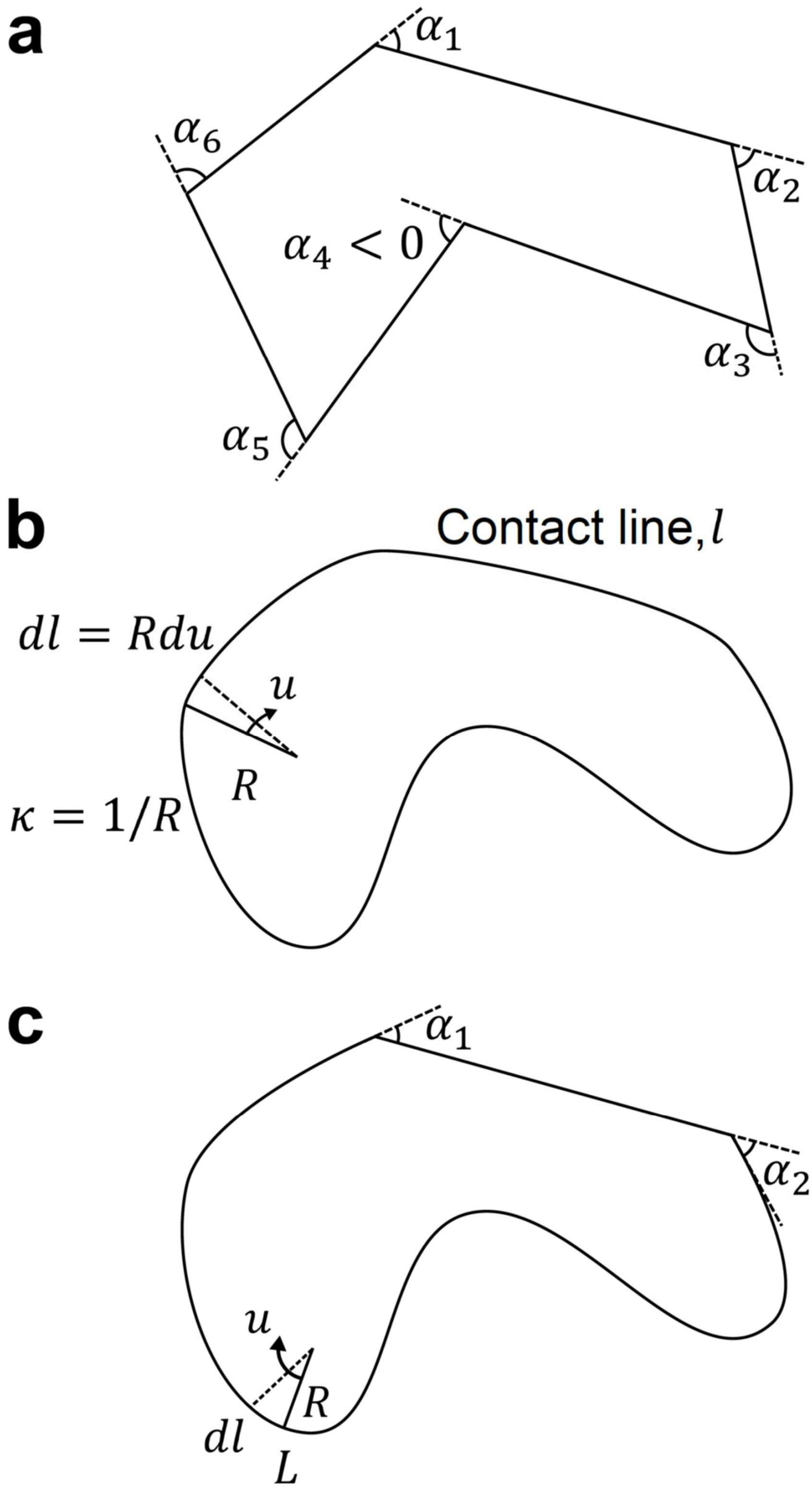

Figure 1. An illustration of angles and curvatures in two dimensions. (a) For a polygon the sum of the external angles α_i is 2π. Note that α_4 in a concavity is negative. (b) For a smooth closed loop the equivalent relationship is that the integral of the curvature around the loop is 2π. (c) For a two-dimensional shape bounded by straight sides, sharp angles and smooth lines, the generalization of the relationship between curvature and angles is given by Eq. (1).

If the surface of the droplet were everywhere smooth, then the integral of the Gaussian curvature would be 4π. However, there is a discontinuity in the curvature at the three-phase contact line (where the two fluid phases meet the solid) and this discontinuity is related to the contact angle θ. Analogous to Eq. (1) there is a relationship between the integral of the Gaussian curvature and the contact angle.

The details of the analysis of topology in three dimensions are a little more subtle, but it is possible to prove the following relationship for each fluid-fluid meniscus:

$$2\pi n(1-\cos(\theta-\phi)) + \int G\, dS_{12} = 4\pi \qquad (2)$$

where θ is the average contact angle along the contact line and *n* is the number of contact line loops that the meniscus forms with the solid (it is 1 in Figure 2). The integral is only over the fluid-fluid meniscus, S_{12} (see Figure 2) assuming that the contact line lies in a plane (this is not always strictly true, but is a reasonable assumption). The angle ϕ is the relative orientation of the solid to the plane containing the contact line.

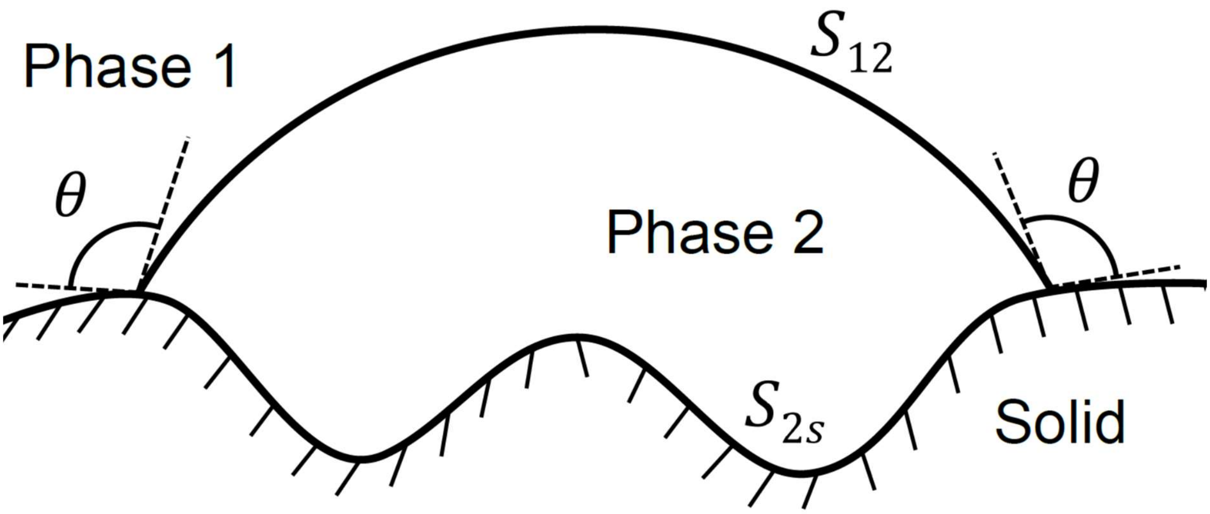

Figure 2. A schematic of a drop of phase 2 on a solid surface surrounded by phase 1. The contact angle θ is shown. We can use Eq. (2) to relate the integral of the Gaussian curvature over the surface S_{12} to contact angle.

To date, the validity of Eq. (2) has been tested on a limited number of datasets – both simulation studies of multiphase flow and images of displacements taken using X-rays: see Figure 3.

There are enormous opportunities for future work. Specifically related to the analysis presented above, we need to assess methods to find the orientation angle ϕ, to quantify the errors associated with assuming that the contact loops lie on a plane, and automatically identifying phases within droplets, since in mixed-wet media we may see both phase 2 surrounded by phase 1 (as in Figure 2) as well as the other way round – phase 1 surrounded by 2. Then the methods need to be tested on a wide range of datasets – both experimental and numerical – to test the accuracy and robustness of the approach.

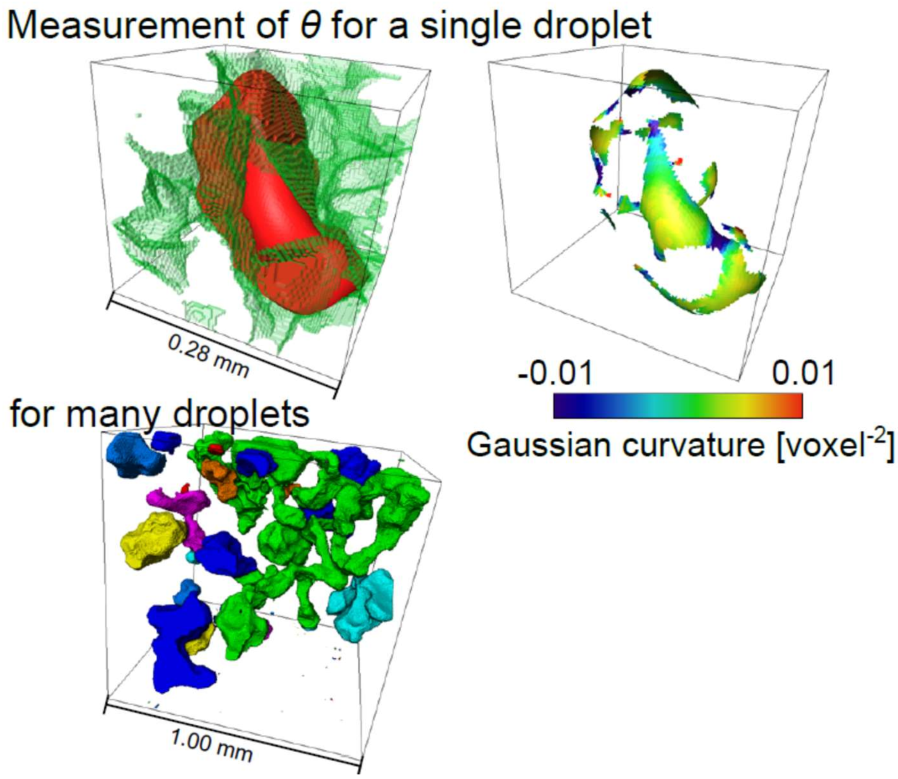

Figure 3. Pore-scale images of phases in a porous medium – the colours distinguish phases, distinct ganglia or the Gaussian curvature of the interfaces. These images can be used to quantify contact angle, θ, using topological principles.

Of particular importance is to use direct numerical simulation of multiphase flow in porous media under different conditions where the input contact angle is known. This provides a good definitive platform to test new ideas and methods, particularly extensions to Eq. (2), or methods to estimate the orientation angle ϕ.

The other strand of new research is associated with the properties needed to assess contact angle, namely areas and curvatures. At present we reply on methods to take a grey-scale image (a quantification of X-ray adsorption) to segment an image into distinct phases, creating a Lego-block type description of fluid configurations. We then identify and smooth interfaces for further analysis. A more elegant solution – which may remove many of the errors and uncertainties in our present analysis – would be to identify interfaces directly from grey-scale images.

Overall this research offers the potential to apply rigorous ideas in mathematics and physics to transform our understanding of multiphase flow in porous materials, with a wide range of important applications.

Who we are looking for. We are looking for a motivated hard-working student with an excellent background in applied mathematics or physical science with an interest in porous media problems. Good mathematical ability and willingness to learn image analysis methods are needed.

Further reading

M J Blunt, T Akai and B Bijeljic, "Evaluation of methods using topology and integral geometry to assess wettability," Journal of Colloid and Interface Science, **576** 99–108 (2020).

M J Blunt, Q Lin, T Akai and B Bijeljic, "A thermodynamically consistent characterization of wettability in porous media using high-resolution imaging," Journal of Colloid and Interface Science, **552** 59–65 (2019).