

## **Review of Pore-Cor Network Modelling Suite v6.00**

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The advance of modelling liquid-structure interactions has been, and continues to be well served by the pore network descriptor Pore-Cor. Its basis of devising a 3D pore structure via pore-throat connectivity has led in many cases to a reappraisal of the dynamics and of the statistical distribution of fluid flow through porous structures. By abandoning the traditional parallel capillary model offered by the direct differential interpretation of porosimetry data, geometrical factors related to dimensional progression, such as that between coarse and fine features, can be evaluated in respect to short timescale phenomena occurring within processes of absorption, permeation, diffusion and filtration, which, in turn, control the average observed behaviour of these phenomena. The value of being able to make the breakdown into local interactions on a pore level provides the means for improved design of functional materials, such as coatings, catalysts, building aggregates, and, for example, in soil mechanics and oil extraction.

In the latest version, the user is introduced to a newly well-ordered display with access to functions appealingly laid out. The length of the access list can give a feeling of foreboding, and perhaps this is well justified, for the model itself has moved on from the restrictions imposed in earlier versions. For example, the limited statistical distribution parameters of pore and throat size via log-linear relations, described by the over-simplified pore and throat skew and linear midpoint pivot, have been replaced by considering the possibility both of banding (correlation) within structures and the additional freedom to consider size spread and skew applied to a bounded distribution. The suite thus provides the tools to follow more informatively the form of the mercury intrusion curve, whilst maintaining realistic all-embracing limits to the size distribution. Care must be exercised, though, when using this newfound interpretative freedom, whilst relation must always be drawn for sound reasoning behind the acceptance of such a wide-ranging parameter field. This is no more clearly illustrated than in the use of the Simplex algorithm to seek an effective combination surface across parameters. It requires the definition of throat skew, throat spread, connectivity, pore skew and correlation level, all of which require a deep knowledge of their impact and a highly educated start point in relation to the structure under investigation, otherwise the model fails to reach a satisfactory result. Fortunately, its designers have built in a self-consistent limiting, which informs all too readily that the start point combination is leading to divergence. It smacks somewhat of the benefit of hindsight, but the stochastic generation of random structures provides a good way to check consistency before venturing to the more exotic. Nonetheless, for the intrepid expert who has evidence of the type of structure under investigation, such as images from microscopy or even tomography, the adventure is highly rewarding, as features, such as micro-orientational inhomogeneity, filter bed build-up and structure consolidation, can be tracked. Given the added ability to apply meniscus forces using the fast wetting algorithm based on Bosanquet inertia, itself equally applicable to de-wetting, permits forces exerted within the structure, themselves leading to structure deformation, to be derived.

The biggest disappointment remains the delivered absolute value of modelled permeability. In its favour, however, this function has been shown in many experimental cases to track reliably the experimentally observed values, but nearly always with a distinct under estimation. Remove the units and call it relative permeability and the user will learn to find this a valuable indicator. It remains to be seen whether tortuosity will prove to be a good descriptor, and perhaps provide an alternative to the Dinic pathway-derived permeability. The addition with most potential is likely to be the description of diffusivity, especially in the case of complex dual porosity structures. Those involved in catalyst design, moisture boundary control, evolution of aroma, drug carrier properties, and the like, should not miss this opportunity to seek better solutions provided from the understanding of pore networks that the model provides.

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