










STATIC ELASTIC PROPERTIES OF ROCKS OBTAINED BY X-RAY MICROTOMOGRAPHY, INVERSE MODELING AND SURROGATE MODEL

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APPENDIX A

Benchmark of Permeability Estimation

The permeability estimation using Simpleware finite element software was validated using benchmark digital rock samples reported by (1) and available at <https://www.imperial.ac.uk/earth-science/research/research-groups/pore-scale-modelling/micro-ct-images-and-networks/>. The permeability estimations of these different rocks are tracked in the literature using various numerical techniques, including Pore-Network Modeling (1, 3), Finite Difference (2) and Lattice Boltzmann methods (1).

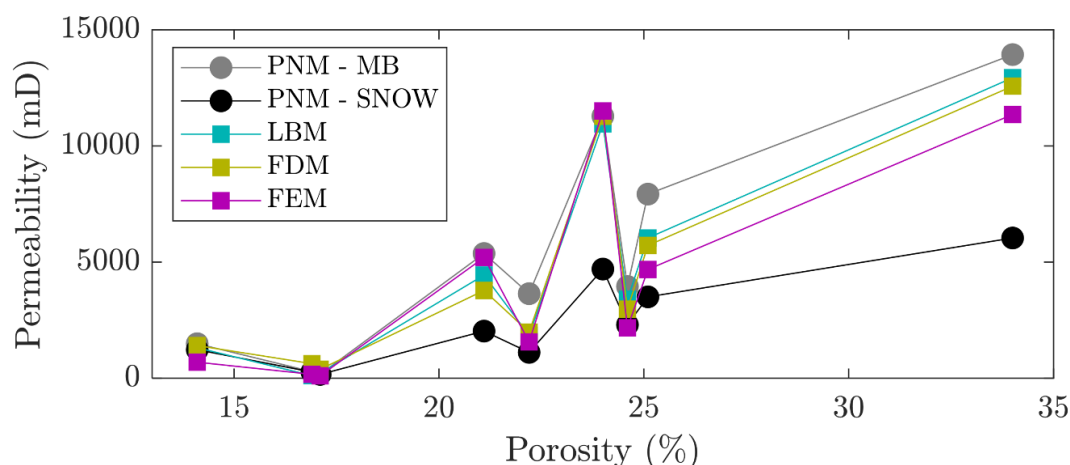


Figure 1: Permeability estimations of the literature database provided by (1), which has been widely explored by different numerical techniques. These techniques are Lattice Boltzmann method (LBM), Finite Difference method (FDM), and Pore Network modelling using two discretization procedures, namely, Maximum Ball (MB), and Subnetwork of the Oversegmented Watershed (SNOW). The Finite Element Method (FEM) was estimated using the Simpleware software and FLOW module in the present study.



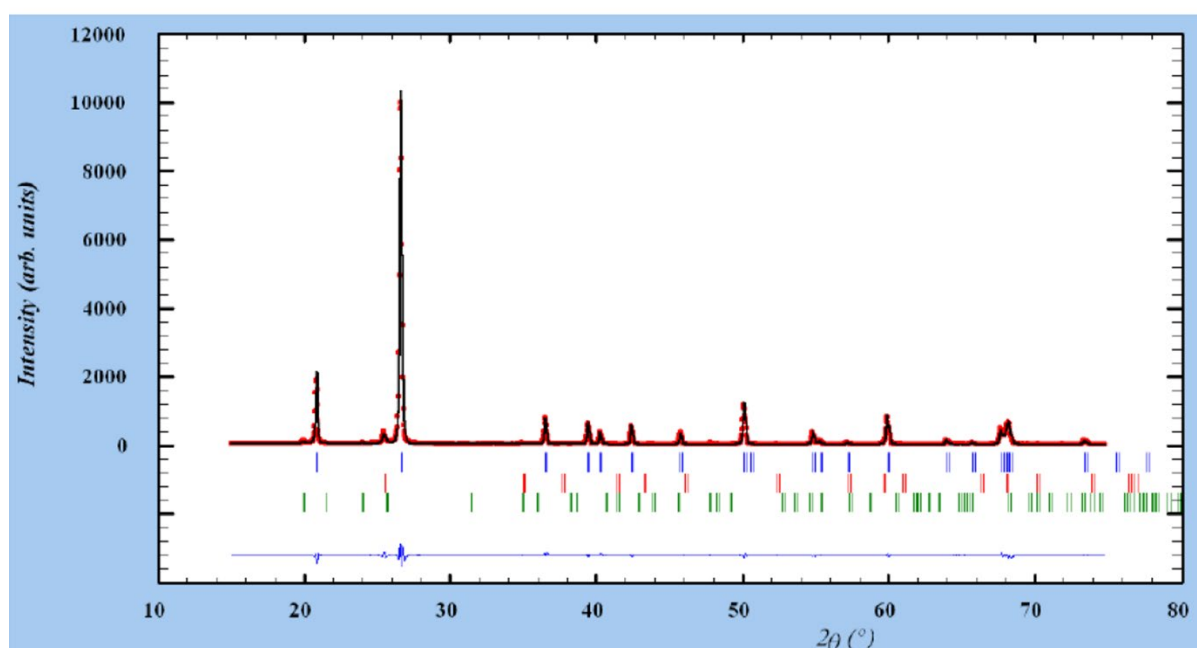


Figure 2: X-ray diffractograms were obtained for the representative sample of the Botucatu Sandstone. The characteristic peaks observed correspond to the typical crystallographic planes of quartz (SiO_2), corundum (Al_2O_3), and heterosite/purpurite (FePO_4), confirming the presence of these crystalline phases in the sample.

Procedure to integrate Abaqus Finite Element software mechanical output solutions into parameter estimation using Matlab

Algorithm 1: Converting, executing, and storing results from Abaqus in Matlab

Script 1: Converting .inp file into Matlab version

Requires pre-processing in Abaqus software

1. Input .inp file
2. Copy each row into a new Matlab file
3. Set a flag to locate and modify Elastic properties
4. Output executable Matlab version

Script 2: Executing numerical simulation through Matlab

5. Input user-defined elastic properties values for each phase
6. Execute Abaqus from Matlab
7. Output simulation files

Script 3: Processing and storing simulation results

8. Input simulation files
9. Access Output elements and post-process stress-strain
10. Output vectors with stress-strain and adopted Elastic properties.

References

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2. Gerke K, Vasilyev RV, Khirevich S, et al. (2018). Finite-difference method Stokes solver (FDMSS) for 3D pore geometries: Software development, validation and case studies. *Computers and Geosciences* 114, 41–58. <https://doi.org/10.1016/j.cageo.2018.01.005>
3. Gerke K, Sizonenko TO, Karsanina M, Lavrukhin EV, Abashkin V, et al. (2020). Improving watershed-based pore-network extraction method using maximum inscribed ball pore-body positioning. *Advances in Water Resources*, 140, 103576. <https://doi.org/10.1016/j.advwatres.2020.103576>