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Numerical modelling based saturation conductivity estimation uncertainty – influence of the quality of the pore space geometry representation based on X-ray CT images

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Introduction

Saturated water conductivity (SWC) may be estimated based on simulations of the single phase fluid flow in pore media. Such approach is used for years in geophysical, petrochemical and other applications. The obvious role in this approach has proper description of the pore medium. X-ray computational tomography (CT) is routinely used for gathering information about pore space geometry. CT scans quality - mostly in terms of resolution and voxel size - was recognized already as a factor influencing results of the saturated conductivity simulations.

As the SWC is estimated by the numerical simulations, one may expect that numerical mesh quality may have impact on the simulated water conductivity values. Generated mesh should follows exactly pores geometry. Unfortunately any numerical mesh generation procedures can't follow pore-space exactly.

The aim of this study was to asses the mesh quality on the simulated saturated water conductivity.

Ksat estimation from CT images

SWC may be estimated through numerical modelling of the single phase transport in the pore-space determined by the CT scans. In case of this study OpenFOAM software were used for mesh generation (snappyHexMesh tool) and for fluid flow simulations based on solving the Navier-Stokes equations of transport (simpleFoam solver).

The workflow allowing for that consists of following steps:

- CT scan of the pore medium (CT scan voxel size was 2μm),
- Thresholding of the 3D CT image (pore-space is determined at this step),
- Mesh generation in the area of the pore-space,
- Numerical simulation solving N-S equations (pressure and fluid velocity field is determined),
- Calculation of the SWC based in fluid flux and pressure drop on the sample length.

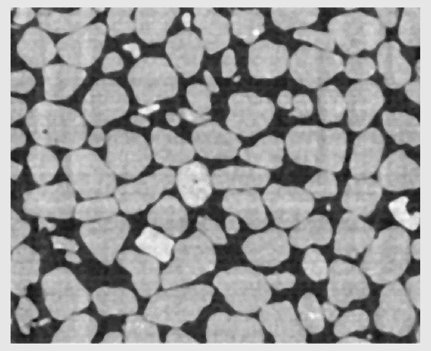

Figure 1: Raw view of the pore media scanned using CT (sample cross-section of 3D CT volume).

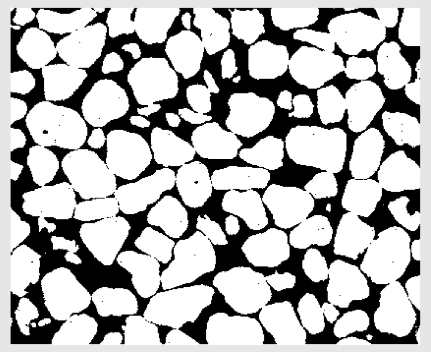

Figure 2: Thresholded CT image distinguishing between pore space and solid phase of the pore medium.

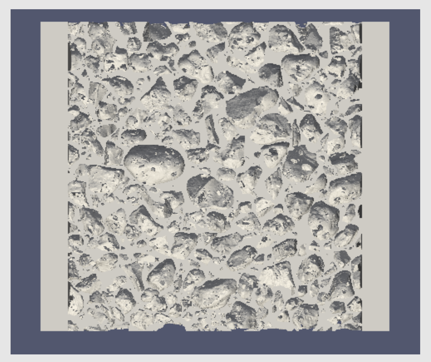

Figure 3: Mesh representing pore-space of the pore medium.

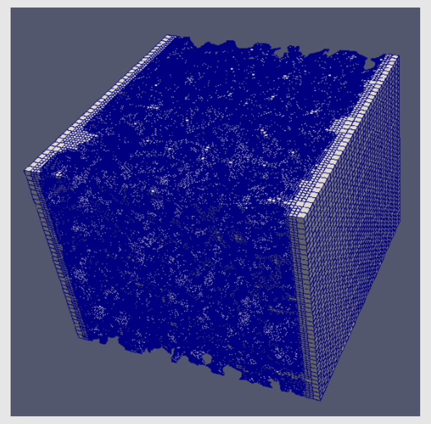

Figure 4: Visualization of the cells in the mesh.

Based on simulations results SWC may be estimated using Darcy's law:

$$K_{sat} = \frac{q\rho g}{\Delta p}$$

where: K_{sat} - saturated water conductivity (SWC) $[m \cdot s^{-1}]$, q - fluid flux $[m \cdot s^{-1}]$, g - standard gravity $[m \cdot s^{-2}]$, ρ - fluid specific density $[kg \cdot m^{-3}]$ and Δp - pressure drop along sample $[Pa \cdot m^{-1}]$.

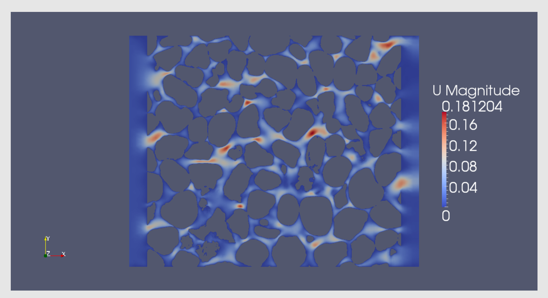

Figure 5: Visualization of the simulated velocity magnitude field in sample cross-section.

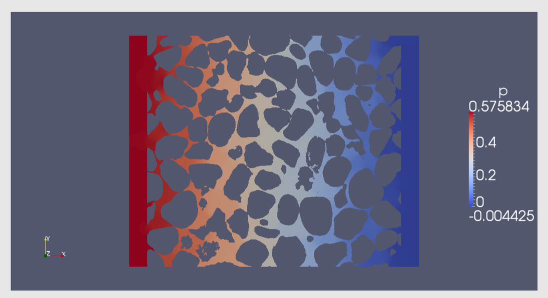

Figure 6: Visualization of the simulated pressure field in sample cross-section.

Mesh generation & quality issues

Mesh quality is always an important issue in numerical calculations. Dependently on numerical method of equations discretization, different mesh quality measures will be important. OpenFOAM simulation package is based on Finite Volume Method (FVM) discretization scheme. In case of FVM typical mesh quality measures are among other: cell skewness and cell aspect ratio. During mesh generation procedure, when cells are cut and fitted to complicated pore-space geometry, some cells might not meet quality assumed criteria. In case of this study, these cells were simply removed from mesh. Removed cells were not numerous and its removal didn't influence simulations.

"Mesh quality" as understood in this work means - "How well pore-space geometry is followed by the numerical mesh". One of the most important mesh characteristics is minimum dimensions of cell which could be achieved. Of course the smallest cell, the better - because pore geometry will be followed more exactly by the mesh. But there is important tradeoff between minimum cell size and technical resources (CPU time, RAM size needed) needed for mesh generation. In practice resources needed for mesh generation may limit possible minimum mesh cell size.

Minimum cell size could be determined differently when snappyHexMesh tool is used form mesh generation. For the purpose of this work it was determined solely by the initial mesh cell size. As the initial cells was split up to 5 times near pore surface during mesh generation, the size of initial cell determines final size of minimum cell - see the table.

mesh ID	init cell size [mm]	min. cell size [μm]
m10	0.4	12.5
m20	0.2	6.25
m30	0.1	3.125
m40	0.05	1.5625

Table 1: The dependence between initial cell size and minimum cell size for investigated meshes.

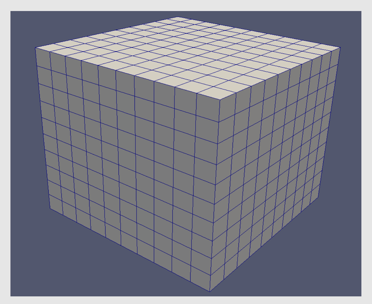

Figure 7: Cell division in initial m10 mesh generation step (10x10x10 cells).

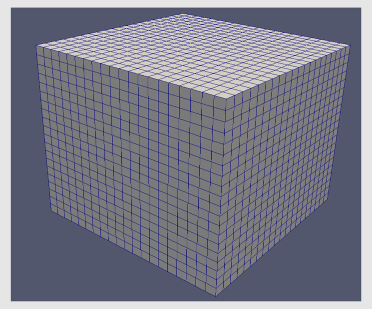

Figure 8: Cell division in initial m20 mesh generation step (20x20x20 cells).

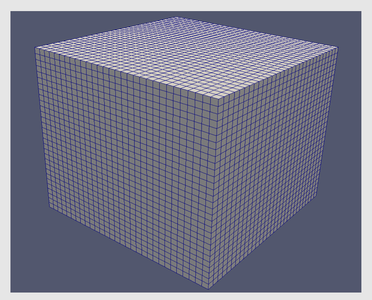

Figure 9: Cell division in initial m30 mesh generation step (30x30x30 cells).

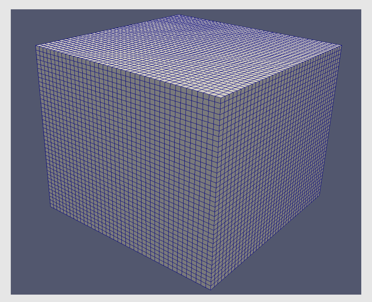

Figure 10: Cell division in initial m40 mesh generation step (40x40x40 cells).

The minimum cell size for the coarsest mesh m10 is ~16μm while the mesh m4 reaches minimum cell size ~1.5 μm which is slightly below CT resolution which was 2μm.

One may expect that in case of coarse mesh m10 only wider pore channels will be meshed. On the other hand mesh m40 reaching with the minimum cell size the voxel size used in CT in principle should recover any pore-space geometry.

Mesh generation & quality issues - cont.

Investigated in this work pore media were 4mm in diameter and height samples prepared from three sieved sand fractions: s1a, s1b 0.32-0.5mm; s2a, s2b 0.16-0.32mm; s3a, s3b 0.8-0.16. Remaining 4 samples s4a, s4b, s5a and s5b were prepared two different sandstones.

Visible below on following figures sample cross-sections of the same region extracted from the mesh show how details of pore-space geometry are represented by meshes with different size of minimum cell.

It may be observed that in case of the coarsest mesh m10 substantial parts of the pore-space was not meshed. Meshing couldn't proceed in pores narrower than relatively big minimum cell size threshold - 16 μm. In case of mesh m20 majority of the pore-space was meshed, while in case of m30 and m40 meshes virtually all pore-space is filled up by the mesh.

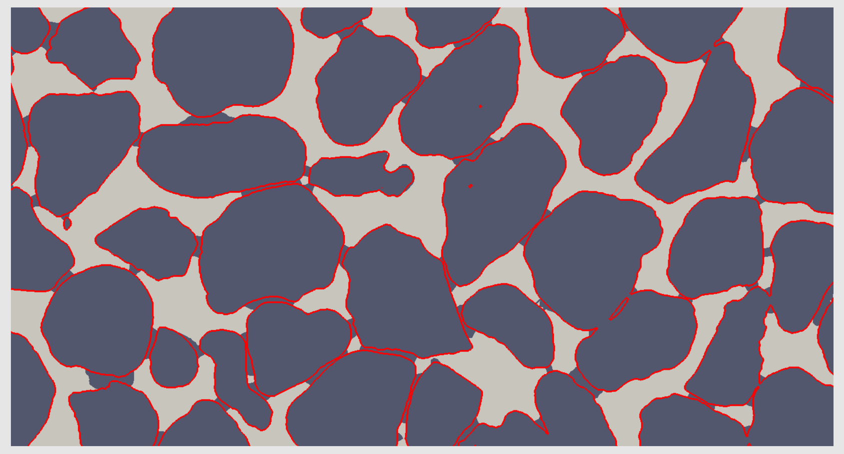

Figure 11: Detail of generated m10 mesh (red lines - true geometry, beige - meshed area/pore, gray area - not meshed area/solid).

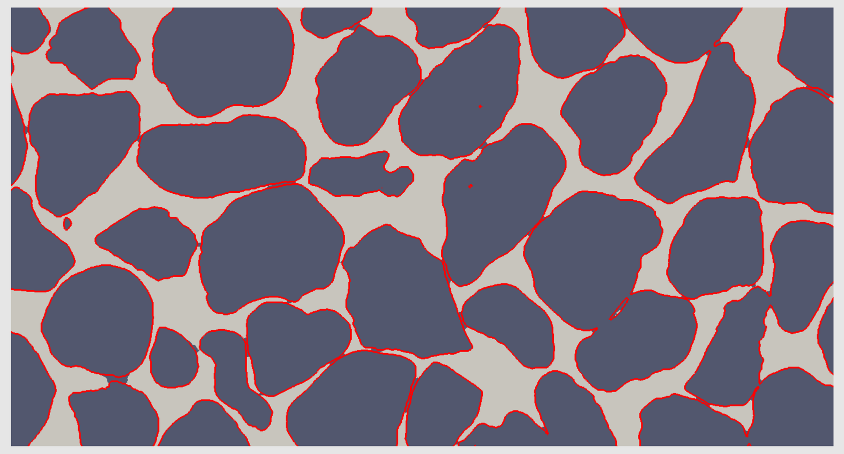

Figure 12: Detail of generated m20 mesh (red lines - true geometry, beige - meshed area/pore, gray area - not meshed area/solid).

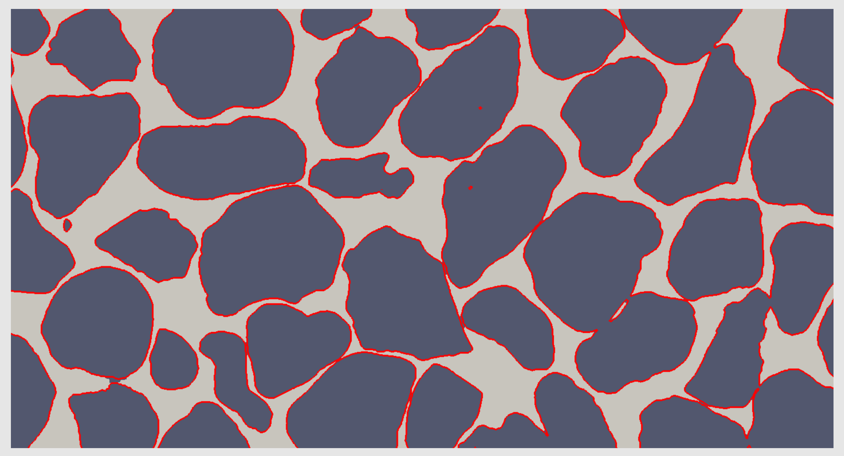

Figure 13: Detail of generated m30 mesh (red lines - true geometry, beige - meshed area/pore, gray area - not meshed area/solid).

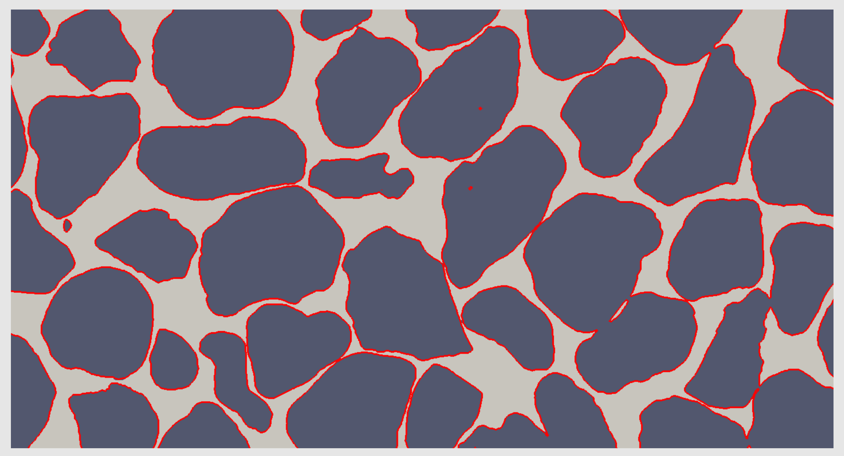

Figure 14: Detail of generated m40 mesh (red lines - true geometry, beige - meshed area/pore, gray area - not meshed area/solid).

Results

Following figure shows pore media specific surface as recovered by the mesh generated in relation to exact specific surface read from the tomographic images. Tomographic image specific surface was treated as a reference. Correct value of relative specific surface would be exactly 1.0. Which would mean that for mesh it is exactly like for thr CT image which was used for mesh generation.

One would expect that if meshes do not follow pore-space exactly the specific surface and total porosity determined for meshes will be lower than true values for CT images.

It might be observed that the coarsest mesh, the lower is the value of specific surface of the mesh. Mesh with bigger value of minimum cell size can't be generated in narrow area of the pore-space. The surface of the pore-solid interface (Figure 15) and the volume of the pore-space (Figure 16) will be lower in that case.

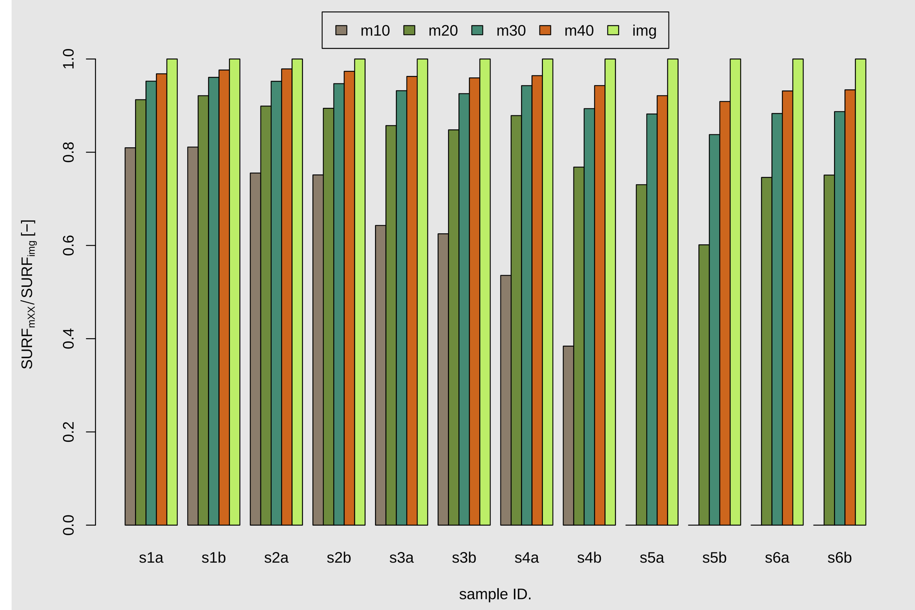

Figure 15: Specific surface of the mesh in relation to true specific surface of a pore media as determined by CT.

Total porosity is another pore-space important characteristics. In this work total porosity of the generated mesh was also determined. It is compared with "true" value of the total porosity i.e. determined for the CT image of the pore-space (Figure 16).

Similarly to specific-surface coarsest meshes underestimate total porosity for the same reasons.

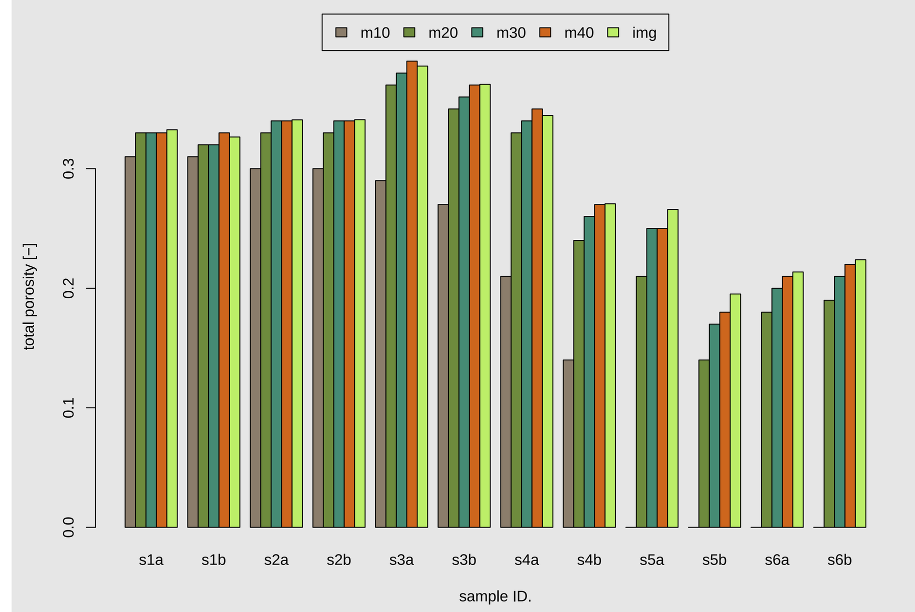

Figure 16: Total porosity of the mesh and a pore media as determined by CT.

For all samples there were attempts to generate all four meshes (m10, m20, m30 and m40). But in case of samples s4 and s5 - which were samples of sandstone material the most coarsest mesh m10 couldn't be generated at all. In that case mesh generating procedure proceeded to mesh spaces where pores were too small for minimal cell to be fit in and mesh generation stopped presumably (Figure 17).

Results - cont.

Correctly generated mesh spreading across all scanned pore medium is presented on Figure 18.

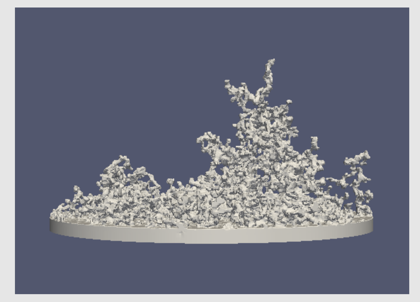

Figure 17: Part of failed m10 mesh generated for s4 pore medium.

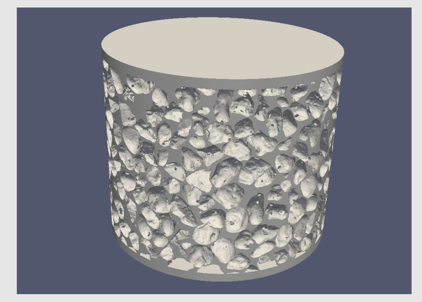

Figure 18: Correctly generated mesh for s1a sample.

Major result form presented analysis is quantification of the mesh quality on estimated value of the saturated water conductivity (Figure 20). As a reference here estimated for finer mesh m40 saturated conductivity was used.

The trends in this case are not so obvious as for specific surface and for total porosity. Meshes m10 may overestimate moderately and underestimate strongly estimated saturated conductivity dependently on the type of the pore medium.

Estimations made for two finer meshes m30 and m40 are always close each other.

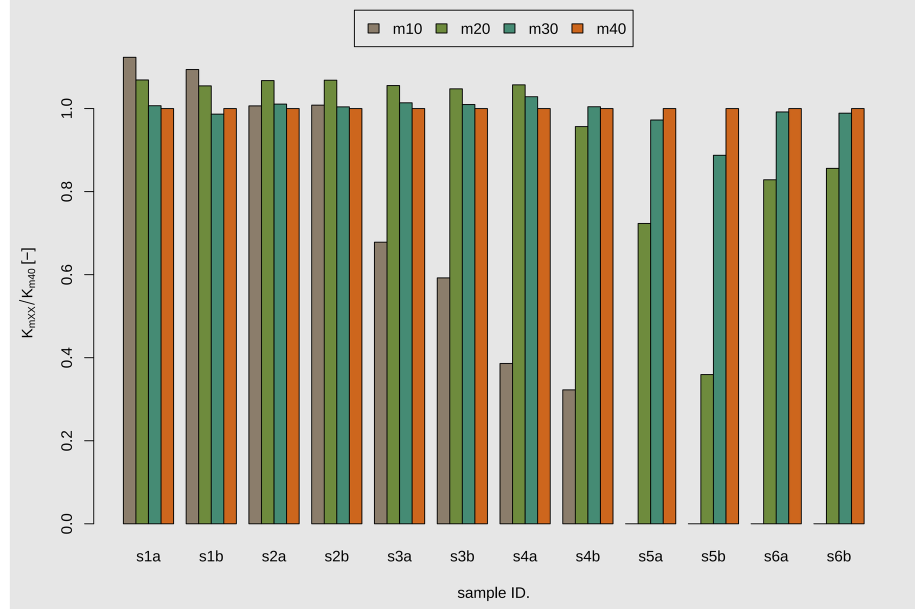

Figure 19: SWC simulated for different meshes in relation to most accurate mesh m40.

Conclusions

- Study showed that the mesh granularity (i.e. size of minimum mesh cell) influences strongly how exactly pore-space geometry is followed by the mesh.
- The best mesh in terms of quality of results was the most finer mesh m40.
- Taking into technical problems facing m40 mesh generation one would point second finest mesh m30 as a good tradeoff allowing for optimal simulation results and still computationally manageable calculational task. In most cases differences in results (Ksat, total porosity, specific surface) obtained by m30 and m40 meshes are meaningless.
- Based on results gathered by this study we may conclude that the minimum size of the cell should be at the level of the CT resolution used for pore media scanning.
- In conducted study saturated conductivity most diverse differences in estimations were: overestimation by 20%, and underestimation by 60%.

Acknowledgments

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