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Contribution ID: **702**   Type: **Oral Presentation**

Multi-scale imaging and modelling for reactive diffusion at the pore scale

Wednesday, 2 June 2021 20:05 (15 minutes)

In the frame of a project aiming to develop a multi-scale imaging and modelling procedure for reactive transport in porous media, we present our first results concerning diffusion and reaction. For the problems we consider, heterogeneous reactions are dominant, meaning that the reactive part of the fluid/solid interface must be precisely described at the local scale. On the other hand, the global spatial distribution of the solid must also be precisely characterized because it determines the representativeness of the average transport properties. Multi-scale imaging techniques can provide a "low"resolution image, corresponding to a large field of view, that can be used as input for computing the average transport properties, and "high"resolution images that describe the fluid/solid interface in details. For numerical modelling we need the "low"resolution image of all the computation domain, and "high"resolution information of the zones having a strong effect on the transport, for instance zones where significant reactions take place. Acquiring a "high"resolution image of the full computation domain is not realistic, and, if an average value is not sufficient for modelling (effective reactive surface), we need a way to incorporate in a multi-scale model both "high"resolution and "low" resolution information.

We use an iterative multi-scale numerical modelling approach: After a first simulation at the "low"resolution scale (i.e. relevant for the transport at the global scale), the zones where grid refining is necessary are selected using an error estimate procedure. Local refining can then be used to complement "low"resolution image in these zones and generate finer grid to improve the quality of the results. Different approaches are explored for this refining step. They will be exposed at the end of the presentation.

To be representative, "low"resolution 3D images are generally big. This results in a large number of grid elements and computationally demanding problems to solve. To temper the computation effort, we first perform a coarsening of the initial grid. After describing the algorithm employed to build of a non-uniform Cartesian mesh, consequences of this coarsening step will be presented for a reactive diffusion problem in terms of precision of the computed effective properties and reduction of the computation costs.

Then, the refining step will be presented and the improvements obtained using different strategies will be compared.

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Time Block Preference

Time Block A (09:00-12:00 CET)

References

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