Hybrid modeling of coupled transfer in porous media: possible options for a mechanistic model ”augmented” by machine learning

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Abstract Mechanistic modelling of coupled transfer in porous media is well-established since several decades [1]. The physical formulation at the macroscopic level includes fundamental balance equations supplied by relevant material parameters. At the macroscopic level, a system of three coupled non-linear equation has a high prediction potential. Provided suitable applied mathematics methods are implemented, computational simulations can predict real configurations, including configurations that were not observed before. On the opposite, thanks to their ability to tackle non-linear and dynamics problems, Machine Learning (ML) based model are capable of coping with complex situations even better than mechanistic modelling [2,3]. The main drawback of mechanistic models is their complexity as operational tools, namely in providing the whole set of product characteristics, while the main drawback of ML tools is its restriction to the domain paved by the database. Different pathways can be proposed to merge the best of the two worlds:

- A full coupled method (hybrid model)
- A fully decoupled method (data base populated by mechanistic modeling used for ML)
- A cascade coupling (ML to complete mechanistic outcomes)

This conference will summarize the physics of the mechanistic formulation and then will present the different possibilities of coupling the mechanistic and ML approaches to obtain an ”augmented” mechanistic model, suitable for process optimization or process control. Finally, the extension of this approach to different configurations, such as biotechnological processes, will be drafted.

Keywords: building energy, drying, machine learning, non-linear equations, on-line tuning, processes.

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