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**Surrogate-based Bayesian comparison of computationally expensive models: application to microbially induced calcite precipitation.** (English) Zbl 1477.86031

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**Summary:** Geochemical processes in subsurface reservoirs affected by microbial activity change the material properties of porous media. This is a complex biogeochemical process in subsurface reservoirs that currently contains strong conceptual uncertainty. This means, several modeling approaches describing the biogeochemical process are plausible and modelers face the uncertainty of choosing the most appropriate one. The considered models differ in the underlying hypotheses about the process structure. Once observation data become available, a rigorous Bayesian model selection accompanied by a Bayesian model justifiability analysis could be employed to choose the most appropriate model, i.e. the one that describes the underlying physical processes best in the light of the available data. However, biogeochemical modeling is computationally very demanding because it conceptualizes different phases, biomass dynamics, geochemistry, precipitation and dissolution in porous media. Therefore, the Bayesian framework cannot be based directly on the full computational models as this would require too many expensive model evaluations. To circumvent this problem, we suggest to perform both Bayesian model selection and justifiability analysis after constructing surrogates for the competing biogeochemical models. Here, we will use the arbitrary polynomial chaos expansion. Considering that surrogate representations are only approximations of the analyzed original models, we account for the approximation error in the Bayesian analysis by introducing novel correction factors for the resulting model weights. Thereby, we extend the Bayesian model justifiability analysis and assess model similarities for computationally expensive models. We demonstrate the method on a representative scenario for microbially induced calcite precipitation in a porous medium. Our extension of the justifiability analysis provides a suitable approach for the comparison of computationally demanding models and gives an insight on the necessary amount of data for a reliable model performance.

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#### Keywords:

[microbially induced calcite precipitation](#); [Bayesian model selection](#); [Bayesian model justifiability analysis](#); [arbitrary polynomial chaos expansion](#); [surrogate-based model selection and comparison](#); [surrogate-based Bayesian model justifiability analysis](#)

#### Software:

[BaPC](#); [aPC](#); [TOUGHREACT](#)

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