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TReacLab: An object-oriented implementation of non-intrusive splitting methods to couple independent transport and geochemical software

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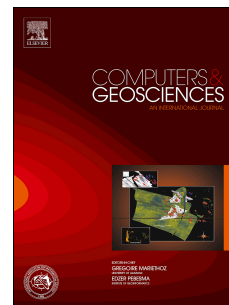
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1 TReacLab: an object-oriented implementation of non-intrusive
2 splitting methods to couple independent transport and geochemical
3 software

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8 **Abstract**

9 Reactive transport modeling contributes to understand geophysical and geochemical processes
10 in subsurface environments. Operator splitting methods have been proposed as non-intrusive
11 coupling techniques that optimize the use of existing chemistry and transport codes. In this
12 spirit, we propose a coupler relying on external geochemical and transport codes with
13 appropriate operator segmentation that enables possible developments of additional splitting
14 methods. We provide an object-oriented implementation in TReacLab developed in the
15 MATLAB environment in a free open source frame with an accessible repository. TReacLab
16 contains classical coupling methods, template interfaces and calling functions for two
17 classical transport and reactive software (PHREEQC and COMSOL). It is tested on four
18 classical benchmarks with homogeneous and heterogeneous reactions at equilibrium or
19 kinetically-controlled. We show that full decoupling to the implementation level has a cost in
20 terms of accuracy compared to more integrated and optimized codes. Use of non-intrusive
21 implementations like TReacLab are still justified for coupling independent transport and
22 chemical software at a minimal development effort but should be systematically and carefully
23 assessed.

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