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Chemical System: An Oriented Object framework applied to reactive transport models

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Reactive transport modelling is becoming increasingly important for the interpretation of the natural and non-natural hydro-geochemical systems. The last decades have witnessed the development of a large amount of reactive transport codes. A problem of this codes is the increasing complexity and the type of programming structure that makes the re-usability of the codes impractical or impossible. For this purpose, we present a new object oriented structure for the organization and manipulation of chemical information that can be used in reactive transport codes. The structure consists of classes that represent chemical species, phases and chemical reactions. The representation of the entire chemical system is encapsulated in a class called Chemical System. The most important characteristics of oriented object concepts are used: (1) encapsulation, (2) inheritance and (3) polymorphism. These characteristics improve, simplify and make more flexible the design of future reactive transport programs. We will show the OOA (Object-Oriented Analysis) and OOD (Object-Oriented Design) of a hydro-geochemical system. Also, we will try to demonstrate that oriented object programming is the proper tool for achieving code modularity.