ABSTRACT

Title: Development of an object-oriented program for solving solute transport equations in porous media

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This document discusses the advantages of object-oriented programming applied to the solution of solute transport equations in groundwater, in absence of chemical reactions. The study has been developed by means of program PROW (PRocess Oriented Groundwater) using FORTRAN90. The PROW program has been designed in the Groundwater section of the Departamento de Ingeniería del Terreno y Cartográfica, in the UPC, using an existent code: TRACONF (programmed in FORTRAN77), which was able to solve transport equations in porous media using the Galerkin finite element method. The worked developed for this document has consisted in adding three new numerical methods: the finite difference method, the method of characteristics (MOC), and the modified method of characteristics (MMOC), which are described in this document. The finite difference method uses a mesh which is different from that used by MEF. Its definitory parameters are fundamentally different, although they are slightly related. MOC and MMOC methods use systems of particles which move with the flow to simulate advection processes. It is needed then to add new concepts to a structure which is designed to solve the finite element method. Due to the different nature of these methods, a way is searched to create the new code in a flexible way, open to changes. Then, object-oriented programming fundamental principles are used. This kind of programming doesn't use a single program flow line, but it consists in an interaction of a series of *objects*, each uno belonging to a *class*. Objects are able to be created, modified or destroyed by means of different methods. These methods, along with a set of properties assigned to each object, describe the so-called class, and define the rules which objects have to follow. There exist some principles for this kind of programming, which are basically: data encapsulation, inheritance and polymorfism. These principles have to be respected as it is possible, in order to get a flexible program in front of changes and incorporations of new code, as well as an information flow constantly controlled and only open to those objects which need it.

Given that FORTRAN90 is not a language designed for this type of programming, some needed techniques are described to simulate it in this language, as well as some tools which it offers for its development: dynamic allocating, modular structures, derived types and INTERFACE sentences. Some design parameters are given also, which were used for the building of PROW. This document makes clear that, in certain cases, not to follow the fundamental rules of this kind of programming can result in an important saving of code burocracy, which is one of the most important problems of object-oriented programming.

Once object-oriented programming is described, it is explained the way PROW works and its structure. It has a MAIN program, which creates the ENGINE object, responsible for the flow program control. For this, it will create and handle different objects, such as meshes, matrixes, time discretizations, flow and transport equations... It is also explained how new code was added to PROW and some problems which were found during this process.

At last, a small solute transport model is solved using PROW, and numerical solutions are compared with analytical one.