Numerical Modelling of the hydrodynamic field coupled to the transport of chemical species through the finite-element method

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We describe the main features of a numerical simulator currently under development for studying water physico-chemical properties during the flooding of hydroelectric plants reservoirs. The work is sponsored by the brazilian Electric Energy National Agency ANEEL and conducted in a joint work of brazilian universities rearchers, with Furnas Centrais Elétricas S. A., the leading brazilian power utility company. An overview of the simulator requirements and of the involved partners is given. The software modules and engineering solutions are briefly discussed, including the finite element based transport module. Some results, future steps and partnerships are presented and discussed.

1 Introduction

The Intergovernmental Panel on Climate Change (IPCC) demonstrated [1] that human activities have changed the atmosphere concentration and distribution of greenhouse and aerosols over the 20th century and at the beginning of the 21th. Altering the natural concentrations of greenhouse gases (GHG) is likely to have significant consequences on the global climate, with an increase in the global mean temperature of $0.3 - 0.6\,K$ since the late 19th century, for example. In this framework, the answers of the scientific and industrial communities are not conclusive on whether the flooding of soils, consecutive to the creation of water reservoirs results or not in a significant anthropic source of GHG emissions. Questions on whether if hydro power plants can be considered a clean energy source are raised nowadays. Currently, almost 90% of the electricity produced in Brazil comes from hydro power plants and the construction of new ones is considered. Environmental concern with potential problems resulting of the extensive use of water resources results in demands for the development of new tools to be used in the management of resources and impact assessment of new reservoirs.

We describe the features of a numerical simulator currently under development in a joint work of Brazilian universities researchers and Furnas Centrais Elétricas S. A., the leading Brazilian power utility company, for studying water physico-chemical properties during the flooding of hydroelectric plants reservoirs. The work is sponsored by the Brazilian Electric Energy National Agency ANEEL.

2 Simulator requirements and engineering solutions

The simulator is developed under the leadership of the Group of Environmental Studies on Hydro Power Reservoirs (GESAR) established at the State University of Rio de Janeiro. Group facilities include laboratories for numerical simulations and for evaluating experimentally the kinetic constants of biomass decomposition, including two ion chromatography. Experiments are conducted in conditions ranging from light exposure and no flow, found at the end of some reservoir compartments, to flow, absence of light and pressurized conditions found in deep zones. All laboratories are now fully operational. Simulator specifications require the development of a robust, user friendly, fast, accurate, expandable and modular software. Expertises involved in the project include ecology, biology, forest engineering, chemistry, fluid mechanics and transport phenomena, computational linear algebra, computational geometry and software engineering.

Engineering tools comprise Object Oriented Programming and XP process (eXtream Programing [2]). A block diagram of the software modules is given in Fig. (1). It comprises a Graphical User Interface (GUI) using OpenGL and a Shell Interpreter. Geographical data in various formats are fed to the *Terrain* module, that generate the level sets and prepare the site geometry for the next module, *Phyto*. Drainage and phyto-physionomy data are added by *Hydro* and handed over to *Mesh*. This module generates the mesh for the transport simulator. Kinetics data on the decomposing biomass is handled by the *decay* module.

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Boundary conditions at the interface with the atmosphere is provided by the *Meteo* module and the results are rendered by *VIS*. The prototype was developed with *Octave* and is currently being rewritten in C++.

The simulator allows for environmental assessment of prospective sites considered for future hydroelectric power plants, including the extent of basin cleaning required and prediction of the water quality. Different compartment of a reservoirs may be individually treated.
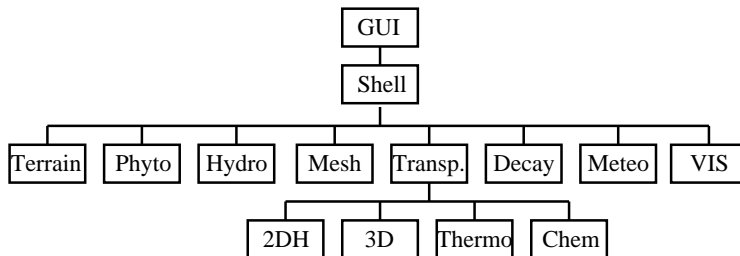
3 The transport simulator and finite element strategies

Fig. 1 Block diagram of the software modules in development at the Group of Environmental Studies on Hydro Power Reservoirs – GESAR (Brazil).

The *Transport* module comprises the core of the simulator, based on a finite element scheme ([3]) and makes use of four additional modules: *2DH* which performs two-dimensional (vertically averaged or laterally averaged) analysis, *3D*, which solves the full three-dimensional transport equations, *Thermo*, which solves the temperature field using the hydrodynamic field from the previous step
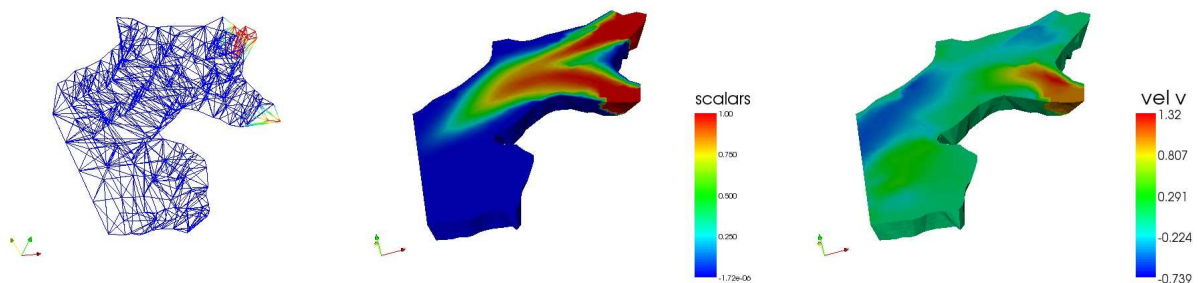
end *Chem*, which deals with the reaction-transport equations of chemical species. Pressure and diffusive terms are treated by a Galerkin method, convective terms are treated in a semi-lagrangean form in order to assure the necessary stability at the code. Time is discretized according to a first order forward differences scheme and the resulting linear systems are solved by a projection method. A reverse Cuthill-McKee reordering and an incomplete Cholesky pre-conditioning schemes are employed to solve the linear systems efficiently. Cubic tetrahedron elements are employed, with the velocity evaluated at the vertices and the centroid of the element. Pressure is evaluated in the vertices only (mini-element). An example of the grid employed in the simulations and of the obtained velocity and the scalar fields shown in Fig. 2.

Fig. 2 An example of the grid employed in the simulations and of the obtained velocity and the scalar fields.

4 Conclusions and future work

Further development of the simulator is currently being discussed with Furnas Centrais Elétricas, to analyze the production, stocking, transport and emission of carbon dioxide and methane in reservoirs and to study fish eggs and larvæ dispersal in reservoirs. Collaboration with the Center for Water Research (Australia), with the National University of Asuncion (Paraguay) and the Brazilian-Paraguayan power utility company Itaipu is also being discussed.

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