APPLICATION OF FINITE ELEMENT METHODS (FEM) IN THE STUDY OF REACTIVE FLOWS

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1 Introduction

1.1 Purpose

To develop prototype computer codes that could allow the mastering of techniques involved in the implementation of FEM to reactive flows.

1.2 Motivation

CH_4 generation from biomass on the bottom of hydroelectric reservoirs, their release in the atmosphere and their potential negative effects as greenhouse gas.

1.3 General description

The construction of large dams to meet the growing energy needs of the country has always been primarily considered due to the fact that very active environmental pressure groups consider this option as being more "clean" and safe that the thermoelectric generation. In reality, the hydropower plants also provide large environmental impact, which can be even more significant that the thermoelectric option because the anaerobic decomposition of organic matter, generating large volumes of greenhouse gases, mainly methane, further exacerbating the problem of global warming. In preparation for a main study, FEM is being used for the numerical investigation of reactive flows in 1D and 2D with application in determination of concentration profiles of chemical species in continuous tubular reactors and degradable pollutants in watercourses. The problem is being studied by solving the transport equation subjected to transient boundary conditions, as it would involve the operation of chemical reactors in diversified production and non-uniform pollutants discharge. By keeping the problem within certain parameters, it was possible to achieve the implementation of a scheme involving the usual spatial discretization for GFEM and Crank-Nicholson for temporal derivative, conveniently dealing with the problems of stability, and a new approach to treat a natural boundary condition.

1.4 Specific situations under consideration

- Determination of species concentration profiles in tubular reactors, where inlet and outlet concentrations of the reactants are constant;
- Determination of species concentration profiles in tubular reactors, where the inlet concentrations are transient and the outlet condition represents a condition of physical-chemical equilibrium;
- Determination of pollutants concentration profiles in waterways, with inlet transient condition and an outlet condition that represents a physical-chemical balance.

2 Numerical techniques

The method has been applied in accordance with the Galerkin model and the resulting integrals of weak formulation were evaluated by the Gaussian Quadrature. The programs generated structured triangular and square meshes. The results were checked with one-dimensional analytical solutions available.

Experimentation with the material derivative as boundary condition at the outlet, i.e.,

$$\left[\frac{\partial C(x_i,t)}{\partial t} + \bar{u}_{x_i}\frac{\partial C(x_i,t)}{\partial x_i}\right]_{\Gamma_{\text{out}}} = 0 \tag{1}$$

Which is equivalent to the weak form as follows:

$$\begin{aligned}
&\sum_{j=1}^{NN} \left(\int_\Omega S_i S_j d\Omega + \frac{D}{U}\int_\Gamma S_i S_j d\Gamma\right)\frac{dC_j}{dt} + \\
&+\sum_{j=1}^{NN} \int_\Omega S_i\left(\bar{u}_x\frac{\partial S_j}{\partial x} + \bar{u}_y\frac{\partial S_j}{\partial y}\right) d\Omega C_j + \\
&+\sum_{j=1}^{NN} \int_\Omega \left(D_x\frac{\partial S_i}{\partial x}\frac{\partial S_j}{\partial x} + D_y\frac{\partial S_i}{\partial y}\frac{\partial S_j}{\partial y}\right) d\Omega C_j + \\
&+\sum_{j=1}^{NN} \int_\Omega k S_i S_j d\Omega C_j = 0
\end{aligned} \tag{2}$$

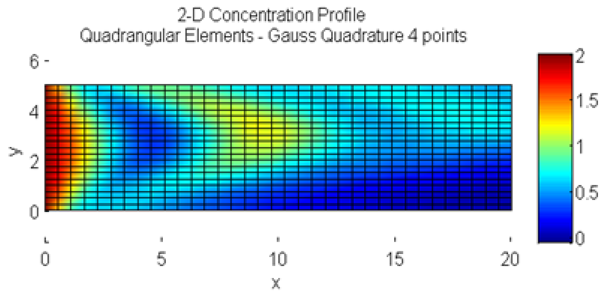
This implies in a modified mass matrix, first term on the left, corrected by the boundary surface integral, and a stiffness matrix modified by the term of reaction, i.e.,

$$[\mathbf{M}_1] \left\{ \dot{\mathbf{C}} \right\} + [\mathbf{K}_1] \left\{ \mathbf{C} \right\} = 0 \tag{3}$$

For its solution, Crank-Nicolson Method and existing criteria to address possible instabilities are applied.

3 Results

The following figure shows an example of a reactive flow simulation with two-dimensional fully developed parabolic speed profile, obtained with boundary condition given by eq.1.



4 Conclusion

The use of FEM is feasible to develop models that can simulate chemical species concentration profiles in reactive flows. The Material Derivative as balancing condition on outlet, represent more faithfully the physical problem and does not induce greater instability. The application of these models in the simulation of the evolution of methane from the bottom of reservoirs of hydroelectric plants can provide ways to capture this gas on the surface and mitigate adverse environmental effects.