

SIMULATION OF A MOVING BED REACTOR USED IN THE PULP AND PAPER INDUSTRY

EXECUTIVE SUMMARY

This project gathered a group of experts in mathematics and chemical engineering to model and simulate numerically the dynamical behavior of a moving bed reactor, the so-called digester, used in the pulp and paper industry. The main goal was to develop a software package, based on innovative numerical methods, to simulate experiments that could be expensive or risky in an industrial context.

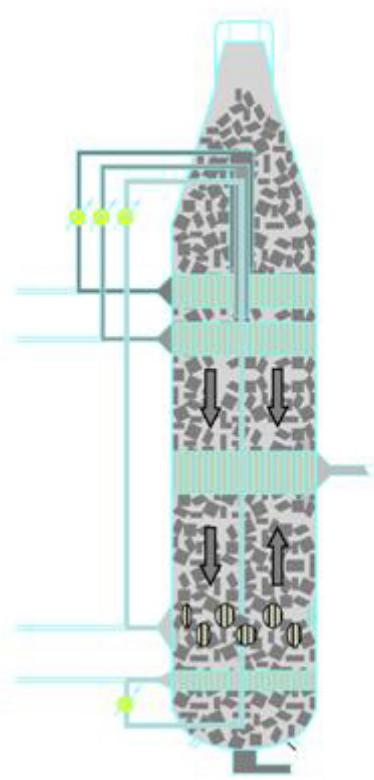
CHALLENGE OVERVIEW

The pulp and paper business is one of Portuguese most important industries. Near Coimbra is located an important mill of the major Portuguese firm Portucel, which is one of the world's biggest producers of bleached eucalyptus Kraft pulp for the packaging industry and one of Europe's top five producers of uncoated wood-free paper. The most critical piece of equipment in a Kraft pulp and paper plant is the digester, known as the heart of the mill. It is a very special and complex heterogeneous reactor where a moving bed of wood chips contacts and reacts with sodium hydroxide and sodium sulphide in a liquid phase (Kraft process), in order to dissolve lignin and therefore to release the fibers of cellulose. In order to optimize the quality of the pulp, this industry has a real need for tools that enable the simulation of experiments that cannot be afforded or that might be risky in a real industrial context.

The problem was tackled under the scope of a research project financed by the Portuguese Science Foundation. The project involved two chemical engineers, five mathematicians and three graduate students, and it was accomplished in three years. The incidence of the work was twofold: from an engineering point of view, the description of the transient behavior of the digester which allows the prediction of the quality of the pulp when some changes in the wood properties occur; from a mathematical point of view, the project gave the possibility to study new numerical methods, specially tailored to the phenomena that take place in each part of the digester.

THE PROBLEM

The dynamical behavior of the reactor can be represented by a system of hyperbolic nonlinear partial differential equations. Among the equations of the system, we can identify three main types: the equations that describe the temperature and the concentration of the solid, the entrapped liquid, and the free liquid phase. Each one of these types of equations presents a certain complexity, making its numerical simulation a hard task. Several factors contribute to the complexity in the numerical simulation: (i) the high nonlinearity of the functions that represents the chemical reactions; (ii) the discontinuities induced by the extraction, enrichment and heat of the free liquor; (iii) the discontinuities in the convection velocity of the free liquor - positive where the liquid flown downwards and negative where the free liquid flows upwards.



Digester

RESULTS AND ACHIEVEMENTS

An open-source software package to simulate the dynamical behavior of the digester was developed and is available by request. This package was tested by the company to simulate the steady-state case with very promising results. The scientific activity is reflected in five papers in international journals and one PhD thesis.

The translation of the mathematical technology into practical terms and its efficient implementation in applicable paradigm is not straightforward. To enhance the process of communication between academia and industry there is a need for academic careers in industrial mathematics to demonstrate the complexity and value of application-driven research.

RESEARCH TEAM

Adérito Araújo, LCM-CMUC

José Augusto Ferreira, LCM-CMUC

Maria Fernanda Patrício, LCM-CMUC

Paula de Oliveira, LCM-CMUC

Paulo Rosa, LCM-CMUC

J.A. Castro, Department of Chemical Engineering, FCTUC

Natércia Fernandes, Department of Chemical Engineering, FCTUC

WEB: <http://www.uc.pt/uid/lcm/projects>