4th CI²MA Focus Seminar
"Polymers and numerical methods for chemical engineering"

May 30, 2013
Auditorio Alamiro Robledo
Facultad de Ciencias Físicas y Matemáticas
Universidad de Concepción

Organizers: Ricardo Oyarzúa and Mauricio Sepúlveda

Programme

9.00 **Opening**

9.05 **Raimund Bürger** (CI²MA-UDEC):
On the Lax-Friedrichs scheme for a transport-adsorption model of polymer flooding in oil reservoir engineering.

9.35 **Patricio Pérez- Guerrero** (DIMAD- UBB):
Modificación de Lignina Kraft para uso en mezclas de Poliolefinas.

10.05 **Erwan Hingant** (CI²MA-UDEC):
An introduction to some mathematical models in polymers science.

10.35 **Coffee break**

11.00 **Christian Núñez** (Departamento de Química, UBB):
Polímeros biodegradables de PLA y PHB a partir de residuos industriales.

11.30 **David Mora** (DMAT-UBB and CI²MA-UDEC):
A locking-free finite element method for Timoshenko beams.

12.00 **Mario Núñez** (CBN-UBB):
Development of wood plastic composites through Radiata Pine and Polypropylene for design and manufacture of windows used in chilean housing.

12.30 **Mauricio A. Sepúlveda** (CI²MA-UDEC):
Numerical methods for a porous medium problem

13.00. **Lunch break**

15.00 **William Gacitúa** (CBN-UBB):
Relación entre propiedades a nanoescala y a mesoescala para madera de Eucalyptus nitens.

15.30 **Ricardo Oyarzúa** (DMAT-UBB and CI^2MA-UDEC):
A numerical method for an incompressible nonisothermal fluid flow problem.

16.00 **Interdisciplinary Meeting**

21.00 **Seminar Dinner**

Practical information

Seminar participants who would like to join dinner should register with CI^2MA secretary:

Ms Angelina Fritz
CI^2MA, office 24
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Abstracts

On the Lax-Friedrichs scheme for a transport-adsorption model of polymer flooding in oil reservoir engineering

Raimund Bürger[1]

We use a Lax-Friedrichs-type of finite difference scheme to prove an existence theorem for the following 2×2 system of conservation laws:

$$\begin{aligned} s_t + f(s,c)_x &= 0, \\ \left(sc + a(c)\right)_t + \left(cf(s,c)\right)_x &= 0, \end{aligned} \qquad (1)$$

where $(x,t) \in \mathbb{R} \times \mathbb{R}^+$; $s(x,t)$ and $c(x,t)$ are the unknown functions. The system (1) is augmented by the initial conditions

$$s(x,0) = s_0(x), \qquad c(x,0) = c_0(x), \quad x \in \mathbb{R}. \qquad (2)$$

Here $s_0(x)$, $c_0(x)$, $a(c)$, and $f(s,c)$ are given functions.
The system (1) was originally motivated by a model for polymer flooding in an oil reservoir [4, 5]. In this model, the variable s is the saturation of the wetting phase, $1 - s$ is the saturation of the oil phase, and the variable c represents the concentration of the polymer in the wetting phase. The function $a(c)$ models the adsorption of the polymer by the rock. This system can be understood as a generic model of coupled transport and adsorption processes. Its applications also include variants of kinematic sedimentation and transport models. When the adsorption term is not present, (1) can be converted by a change of variables to a single scalar conservation law with a discontinuous flux, and existence can be established using known results for equations of that type [3]. For (1), this approach does not seem possible. Our Lax-Friedrichs scheme, along with the analysis used to prove convergence, is an extension of the algorithm and analysis appearing in [2]. In that paper, the authors dealt with a single scalar conservation law with a flux function that varied discontinuously in both space and time. The results of numerical analysis are illustrated by numerical examples for several scenarios [1, 5].

This presentation is based on joint work with Kenneth H. Karlsen (Centre of Mathematics for Applications (CMA), University of Oslo, Norway) and John D. Towers (MiraCosta College, Cardiff-by-the-Sea, USA).

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Modificación de Lignina Kraft para uso en mezclas de Poliolefinas

Patricio Pérez- Guerrero [1]

La lignina es un polímero presente en grandes cantidades en células de plantas y en madera. Es el segundo polímero natural mas abundante después de la celulosa. Esta molécula es compleja y es ampliamente aceptado que la biosíntesis de lignina se produce de la polimerización de tres tipos de unidades de fenilpropano llamadas también monolignoles [1]. Esas unidades son alcohol coniferílico, sinapilico y p-cumarílico. Las tres estructuras se muestran en la Figura 1.

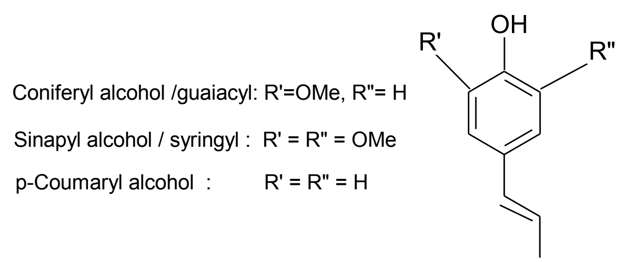

Figura 1. Unidades de monolignoles presentes en ligninas

Numerosos estudios se han realizado para utilizar lignina no modificada como estabilizador y antioxidante de polímeros con resultados contradictorios. El principal objetivo de este estudio se orientó a la modificación química de lignina proveniente del licor negro de procesos Kraft de pulpaje de madera de una mezcla de Eucaliptus globulus y Eucaliptus nitens y estudiar sus efectos sobre los parámetros de extrusión, propiedades físico-mecánicas y térmicas de materiales compuestos a base de poliolefinas recicladas. Se realizaron dos tipos de esterificacin de lignina: con anhídrido acético y con anhídrido maleico. Se analizó los cambios estructurales en lignina esterificada mediante FT-IR, su estabilidad térmica mediante TGA y los cambios en su morfología mediante SEM. La lignina acetilada presentó mayor estabilidad térmica, por lo cual se estudió su efecto en las propiedades térmicas y mecánicas de poliestireno reciclado

Esta presentacion está basada en un trabajo en conjunto con Justo H. Lisperguer (Centro de Investigación de Polimeros Avanzados, CIPA. R08C1002).

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An introduction to some mathematical models in polymers science

Erwan Hingant[1]

The modeling of polymers dynamic involves various mathematical models. Here we want to show an overview of diferent strategies of modelization. We will present the classical size structured model, in its discrete an continuous form. These equations apply to several fields of applications (Biological polymers, Clusters formation, etc) and take into account phenomena such that polymerization, fragmentation and coagulation. Then we will present more complex features, namely, we will assumed the size strucuted equations considering first, an homogeneous space and then inhomogenous. This latter imply to describe the configuration of the polymers and the surrounding fluid interactions. Finally, as a particular example, we finish this talk establishing a system, modeling polymers - metal ions interactions in the context of chemistry.

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Polímeros biodegradables de PLA y PHB a partir de residuos industriales

Christian Núñez Durán[1]

La transformación de la plataforma petroquímica actual por una plataforma biotecnológica basada en el aprovechamiento de la biomasa puede estar enfocada a reemplazar los productos directamente derivados del petróleo o a utilizar los grupos funcionales de los componentes de la biomasa para desarrollar productos nuevos con mejores propiedades y nuevas aplicaciones. La naturaleza produce la mayor parte de las 170109 toneladas de biomasa cada año por el proceso de fotosíntesis, 75% de las cuales pueden asignarse a carbohidratos. Los humanos sólo aprovechamos el 3-4% como alimento o para procesos no alimenticios. Dos tipos de azúcares estn presentes en la biomasa: las hexosas, entre las cuales la glucosa es la más abundante, y las pentosas, en especial la xilosa. Hay dos maneras de transformar los azúcares a bioproductos: los procesos químicos y los fermentativos. La fermentacin de la glucosa produce varios compuestos que pueden utilizarse como materia prima de productos qumicos tiles en la industria, como los ácidos láctico, succínico, itacónico, glutámico y 3-hidroxipropiónico. Sólo como ejemplo, a continuación se muestran algunos derivados útiles del ácido láctico (Figura 1):

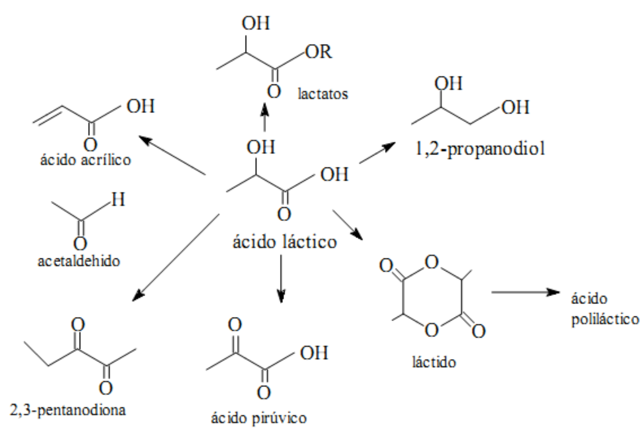

Figura 1. Derivados útiles del ácido láctico.

El proyecto propone innovar en la producción de Poliácido láctico (PLA) utilizando residuos de la industria alimentaria específicamente productos de panaderá que ya cumplieron su vida útil y aprovechar estos residuos en la generación de ácido láctico, materia prima de alto valor. Con la cual se pretende fabricar envases 100% biodegradables para la industria de alimentos produciendo PLA. Evitando de esta forma la competencia en la fabricación de este polímero con los alimentos básicos como la lactosa o amiláceos como el almidón (normalmente de origen vegetal). Además con este proyecto se valorizan los residuos de la industria de alimentos.

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A locking-free finite element method for Timoshenko beams

David Mora[1]

In the present work we study a finite element formulation for Timoshenko beams. It is known that standard finite elements applied to this model lead to wrong results when the thickness of the beam t is small. Here, we consider a mixed formulation in terms of the transverse displacement, rotation, shear stress and bending moment. By using the classical Babuška-Brezzi theory it is proved that the resulting variational formulation is well posed. We discretize it by continuous piecewise linear finite elements for the shear stress and bending moment, and discontinuous piecewise constant finite elements for the displacement and rotation. We prove an optimal (linear) order of convergence in terms of the mesh size h for the natural norms and a double order (quadratic) in L^2-norms for the shear stress and bending moment, all with constants independent of the beam thickness. Moreover, these constants depend on norms of the solution that can be a priori bounded independently of the beam thickness, which leads to the conclusion that the method is locking-free. Numerical tests are reported in order to support our theoretical results.

This presentation is based on joint work with Felipe Lepe (Departamento de Ingeniería Matemática, Universidad de Concepción) and Rodolfo Rodríguez (CI²MA, Departamento de Ingeniería Matemática, Universidad de Concepción)

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Development of wood plastic composites through radiata pine and polypropylene for design and manufacture of windows used in chilean housing

Mario Núñez[1]

The objective of this study was to develop wood plastic composites with suitable properties to be used in the extrusion of windows profiles, appropriate to be installed in Chilean housing in any region of the country. The first stage of this study consisted in the development of wood plastic composites, using: radiata pine sawdust, 10 to 40 mesh size and a 2% moisture content, commercial homopolymer polypropylene, and Struktol TPW-104 lubricant agent. Composites were made using different amount of wood, polypropylene and lubricant agent. The composites were made in a TC-35 Milacron twin screw extruder. The physical and mechanical properties of the composites were evaluated. The second stage of this study included the suitable design of the profiles and dies for the extrusion process of window compounds. The windows were tested in air and water tightness, wind resistance and thermal transmittance, according to Chilean Standard. The results of the study, allowed the development of a wood plastic composites with radiate pine sawdust, polypropylene and lubricant agent, with mechanical and physical properties suitable to be used for the manufacturing of exterior double contact windows. The properties of the windows developed classified in special category in air tightness (10a) and water tightness (30e) tests. In wind resistance test (NCh 888), classifies in exceptional category (20v). Finally, the research allowed the development of a wood-plastic composite, suitable for the manufacture of windows to be installed in Chilean housing in any region of the country.

This presentation is based on joint work with Aldo Ballerini (Centro de biomateriales y nanotecnología, Universidad del Bío-Bío)

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Numerical methods for a porous medium problem

Mauricio A. Sepúlveda [1]

This work is motivated by a combined mixed finite element (MFE) - finite volume (FV) scheme of a two phase flow model for the heap leaching of copper ores modeled by a degenerate parabolic equation
We present some results regarding convergence and error estimate for the finite volume discretization for the porous medium equation

$$\partial_t u - \nabla \cdot (\nabla \beta(u) + F(u)) = r(u), \quad \text{in } Q_T \equiv (0, T) \times \Omega.$$

Initially we have $u(0) = u^0$ in Ω, whereas $u = 0$ on $\partial\Omega$. In the above $0 < T < \infty$ is fixed, Ω is a bounded domain in $\mathbb{R}^d (d \geq 1)$ with a Lipschitz continuous boundary. The function $\beta : \mathbb{R} \to \mathbb{R}$ is non-decreasing and differentiable. By degeneracy we mean a vanishing diffusion, namely $\beta'(u) = 0$ for some u. We prove error estimates for the finite volume discretization for this model. This work was was initially motivated by a a two phase flow model for the heap leaching of copper ores, and have applications in process engineering and wood drying models. Several numerical results illustrating the performance of the algorithm are provided.

This research was partially supported by FONDAP and BASAL projects CMM, Universidad de Chile, Fondecyt 1110540, CONICYT project Anillo ACT1118 (ANANUM), and by Centro de Investigación en Ingeniería Matemática (CI^{2}MA), Universidad de Concepción.

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Relación entre propiedades a nanoescala y a mesoescala para madera de Eucalyptus nitens

William Gacitúa[1]

La Nanotecnología plantea una nueva visión acerca del mundo, esto implica comprender e intentar dominar las propiedades de la materia a escala nanométrica esto es, la mil millonésima parte de un metro, longitud que puede corresponder por ejemplo a un grupo de tomos o incluso alguna pequea molécula. A escala nanom'etrica, la materia ofrece propiedades muy distintas a las conocidas, por eso, la nanociencia posee un carácter transversal a las distintas disciplinas científicas. El objetivo principal de este estudio fue encontrar la relacin existente entre los mtodos de medicin de módulo de elasticidad (E) a mesoescala según la norma ASTM D 143-94 (2006), realizado mediante una maquina de ensayos universales Instron provista de un extensómetro, versus el mdulo de elasticidad entregado por un nanoindentador Triboscope Hysitron Nanomechanical, empleando dos modelos de la micromecánica: la regla de las mezclas y las ecuaciones de Halpin Tsai. Dichos modelos, combinados con correlaciones en base a polinomios de hasta tercer orden, resultaron en una muy buena aproximación entre las propiedades a mesoescala y las propiedades a nanoescala en la especie Eucalyptus nitens.

Este es un trabajo en conjunto con Cecilia Bustos Elías Figueroa (Departamento de Ingeniería en Maderas, Universidad del Bío-Bío).

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A numerical method for an incompressible nonisothermal fluid flow problem

Ricardo Oyarzúa[1]

In this talk we propose and analyze a mixed finite element method with exactly divergence-free velocities for the numerical simulation of a generalized Boussinesq problem, describing the motion of a non-isothermal incompressible fluid subject to a heat source. The method is based on using divergence-conforming elements of order k for the velocities, discontinuous elements of order $k-1$ for the pressure, and standard continuous elements of order k for the discretization of the temperature. The H^1-conformity of the velocities is enforced by a discontinuous Galerkin approach. The resulting numerical scheme yields exactly divergence-free velocity approximations; thus, it is provably energy-stable without the need to modify the underlying differential equations. We prove the existence and stability of discrete solutions, and derive optimal error estimates in the mesh size for small and smooth solutions.

This presentation is based on joint work with Dominik Schötzau (Mathematics Department, University of British Columbia, Canada)

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