



Universidad de Concepción



**Mathematical Modelling for Bioprocesses,
Wastewater Treatment and Mineral Processing**
Third CI²MA Workshop, organized jointly with CRHIAM
Universidad de Concepción, September 27 and 28, 2017
Auditorio Alamiro Robledo, Facultad de Ciencias Físicas y Matemáticas
Organizers¹: Fernando Betancourt & Raimund Bürger

Practical information

People interested in attending the workshop should register with CI²MA secretary:

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Programme

Wednesday, September 27

15.00 Registration and Welcome

Session 1: Models of sedimentation in mineral processing

15.30 **Julio Careaga** (Universidad de Concepción):
Modelling and numerical simulation of sedimentation in conical vessels

16.00 **Manuel Larenas, Pamela Garrido** (Centro de Investigación JRI, Chile):
Numerical simulation of solid-liquid separation
applied to industrial thickening of mining slurries

16.30 **Alonso Pereira, Fernando Betancourt, Fernando Concha,
Daniel Sbárbaro** (Universidad de Concepción):
Process dynamics and control of industrial thickeners

17.00 Coffee break

¹This event is supported by Conicyt projects PFB03 (CMM-Basal), CRHIAM CONICYT/Fondap/15130015, PAI/MEC/80150006, and Fondecyt 1170473.

Session 2: Multi-species systems

- 17.30** **Pep Mulet** (Universitat de València, Spain):
Implicit-explicit conservative schemes
for the equilibrium dispersive model of chromatography
- 18.00** **M. Carmen Martí** (Universidad de Concepción):
Unified multi-class framework to model settling tanks
in water resource recovery facilities
- 18.30** **Diana Celi, Fernando Concha, Christian Goñi** (Universidad de Concepción):
Determination of the volumetric solids fraction
of saturated polydisperse ore tailing sediments
- 20.30** **Workshop Dinner**

Thursday, September 28

Session 3: Flotation, tailings, and slurry flow in mineral processing

- 09.30** **Stefan Diehl** (Lund University, Sweden):
A model of a flotation column described by a conservation law
with multiply discontinuous flux
- 10.00** **Claudia Castillo** (CSIRO Minerals Chile), **Christian Ihle** (Universidad de Chile):
Effect of salinity on the dynamics of flocculation
of copper sulphide tailings with clay content
- 10.30** **Cristian Reyes, Christian Ihle** (Universidad de Chile):
CFD simulation of cation exchange in slurry pipeline flow
- 11.00** **Coffee break**

Session 4: Reactive models

- 11.30** **Elena Torfs** (ModelEau, Université Laval, Québec, Canada):
Full scale measurements and model development
for reactive settling of activated sludge
- 12.00** **Elisa Giustinianovich** (Universidad de Concepción),
José Luis Campos-Gómez (Universidad Adolfo Ibáñez),
Camilo Mejías, Marlene Roedel (Universidad de Concepción):
Granular partial nitrification/Anammox process: why modelling and main challenges
- 12.30** **Camilo Mejías** (Universidad de Concepción):
Modelling biofilm growth in a granular sludge bioreactor
- 13.00** **Closing remarks**

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**MODELLING AND NUMERICAL SIMULATION OF SEDIMENTATION
IN CONICAL VESSELS**

JULIO CAREAGA

ABSTRACT. One-dimensional models to simulate secondary settling tanks (SST) with cylindrical geometry are widely used in wastewater treatment. One of these models is the *Bürger-Diehl model* developed in [3], the respective extension to the varying cross-sectional area case was recently made in [1]. For the modelling, simulation and control of SST according to this model it is necessary to know the hindered-settling velocity function, which is considered a constitutive functions of the model. The traditional way to get this function is to measure the velocity of the declining sludge blanket in a vessel with constant cross-sectional area through experiments obtained from laboratory batch tests, however this method gives only one point on the flux curve. A newly developed method in [2] shows that in a vessel with varying cross-sectional area a large part of the flux function can be estimated from a single batch test, where the largest interval can be obtained with conical vessels.

The identification of the hindered-settling velocity function, a method of determination of the induction period for conical batch tests and simulations using the extended *Bürger-Diehl model* to the varying cross-sectional area case are presented.

This contribution is a joint work with Raimund Bürger (Universidad de Concepción, Chile), Stefan Diehl (Lund University, Sweden), Ryan Merckel (University of Pretoria, South Africa) and Jesús Zambrano (Mälardalen University, Sweden).

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**NUMERICAL SIMULATION OF SOLID-LIQUID SEPARATION
APPLIED TO INDUSTRIAL THICKENING OF MINING SLURRIES**

MANUEL LARENAS & PAMELA GARRIDO

ABSTRACT. The thickening process is a major concern in the treatment of highly concentrated mining slurries. Despite the longstanding multidisciplinary effort to understand the phenomena involved, the industrial operation is still largely based on empirical considerations.

Among the research areas developed at Centro de Investigación JRI (CI-JRI), industrial thickening has gained great attention in recent years due to the scarcity of water resources in Chile and the need to meet increasing production goals. In this Workshop, we present some aspects of numerical simulations based on a well-established mathematical model of solid-liquid separation [1], providing a new approach focused on applications.

The current implementation of the computational simulator is flexible, allowing for exploration on several aspects including, among others, the effects of tank geometry and the settling behavior of the pulp. Common features such as bed height, compression, dispersion and concentration profiles can be observed in batch and continuous mode of operation, showing in general good agreement of the model vs. experimental data. Additionally, we have carried out wide-ranging studies, including the identification of the flux function in conical vessels [2]. This analysis has been used to adjust some of the elements of the mathematical model and assess the predicting capabilities of the simulations.

In association with a mineral processing plant, CI-JRI is currently embarking on an extensive on-site project aimed at gaining insight towards the validation of these tools at industrial scale. The consolidation of this line of work will contribute to the analysis of different operational conditions and provide a better understanding on possible directions to improve water recovery, quality of disposals and general efficiency of the process.

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**PROCESS DYNAMICS AND CONTROL OF INDUSTRIAL
THICKENERS**

ALONSO PEREIRA, FERNANDO BETANCOURT, FERNANDO CONCHA

ABSTRACT. The rational use of water has become an important issue in mining industry, especially in countries located in desert areas with low hydro reserves [1]. Nowadays the need to increase the capacity of many copper concentrators, water scarcity, and high cost of fresh water makes necessary to maximize the recovery of water used in plant, which is done by solid-liquid separation processes. Thickeners work continuously to produce a concentrated underflow, while supernatant water overflows free of particulate matter. The thickening process is highly non-linear and practice has shown that standard feedback control has not been effective in providing consistent operation [2]. In many plants thickeners operate with poor standards, with high dosage of flocculants and highly variable underflow concentration [3]. This article presents: an overview of the current control strategies in mining industry, advances developed in new controllers using phenomenological mode, and instrumentation developed in the University of Concepcion. The analysis of results shows the characteristics of each of the control strategies, and provides suggestions about how to improve their performance.

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**IMPLICIT-EXPLICIT CONSERVATIVE SCHEMES FOR THE
EQUILIBRIUM DISPERSIVE MODEL OF CHROMATOGRAPHY**

PEP MULET

ABSTRACT. Chromatographic processes can be modeled by nonlinear, convection-dominated partial differential equations, together with nonlinear relations: the *adsorption isotherms*. We consider here the nonlinear *equilibrium dispersive* (ED) model with adsorption isotherms of *Langmuir type*. We show that, in this case, the ED model can be written as a system of conservation laws when the dispersion coefficient vanishes. We also show that the function that relates the conserved variables and the physically observed concentrations of the components in the mixture is one to one and it admits a global inverse, which cannot be given explicitly, but can be adequately computed.

As a result, fully conservative numerical schemes can be designed for the ED model in chromatography. We propose a Weighted-Essentially-Non-Oscillatory second order IMEX scheme and describe the numerical issues involved in its application. Through a series of numerical experiments, we show that our scheme gives accurate numerical solutions which capture the sharp discontinuities present in the chromatographic fronts, with the same stability restrictions as in the purely hyperbolic case.

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**UNIFIED MULTI-CLASS FRAMEWORK TO MODEL SETTLING
TANKS IN WATER RESOURCE RECOVERY FACILITIES**

MCARMEN MARTÍ

ABSTRACT. Recent experimental evidences [1, 2] show that variations in distributed particle properties such as size, shape, porosity, density and flocculation state have an important influence on the settling behaviour in different settling unit processes, as primary settling tanks (PSTs) and secondary settling tanks (SSTs). Hence, although each settling process is still governed by its own specific dynamics, these dynamics can be attributed to a common source, thus calling for a unified framework to describe the different settling unit processes.

A unified model framework that considers several particle classes is proposed in [3] in order to describe distributions in settling behaviour as well as the effect of variations in particle properties on the settling process. The result is a set of partial differential equations (PDEs) that are valid from dilute concentrations, where they correspond to discrete settling, to concentrated suspensions, where they correspond to compression settling. The use of a consistent and robust numerical method to obtain well-resolved and reliable approximations to the PDE solutions is discussed in [4].

This contribution is based on a joint work [3, 4] with Raimund Bürger (Universidad de Concepción, Chile), Stefan Diehl (Lund University, Sweden), Pep Mulet (Universitat de València, España), Ingmar Nopens and Sophie Balemans (Ghent University, Belgium), Elena Torfs and Peter A. Vanrolleghem (Université Laval, Canada), Florent Locatelli, Julien Laurent and Pierre François (Université de Strasbourg, France).

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**DETERMINATION OF THE VOLUMETRIC SOLIDS FRACTION OF
SATURATED POLYDISPERSE ORE TAILING SEDIMENTS**

DIANA CELI, FERNANDO CONCHA, CHRISTIAN GOÑI

ABSTRACT. Tailings are mixtures of crushed rock and processing fluids from mills, washers or concentrators that remain after the extraction of economic metals, minerals, mineral fuels or coal from the mine resource [3]. Tailings are sent to the thickening stage to recover part of the water it contains. The bulk of the water is first removed by sedimentation to produce a thickened pulp of about 55–65% solids by weight. The thickened tailings solids are then deposited at the tailings disposal [1, 4]. This work presents a new method to determine the concentration profile of a saturated polydisperse ore tailing sediment without the presence of flocculant in steady state. To this end, a method to resolve the balance of effective solid stress $\sigma(z)$ and concentration profile $\phi(z)$ is developed. It considers a stress distribution in a saturated and static granular medium in equilibrium with the hydrostatic pressure of the surrounding fluid. To resolve the coupled problem $(\sigma(z), \phi(z))$, a new constitutive equation for the volumetric solids fraction is proposed based on the concept of the compressibility of porous material. As a result, a method to estimate the axial concentration and effective stress distribution profile as a function of quantifiable physical parameters is obtained. The solution is validated using a series of experiments consisting of batch sedimentation tests of suspensions at different concentrations. In addition, the model can characterize a specific tailing type through physical parameter k_c . Finally, it is concluded that the effective stress profile obtained by the model is of a non-linear nature, which explains the conventional use of potential or exponential correlations for effective solid stress.

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**A MODEL OF A FLOTATION COLUMN GIVEN BY A
CONSERVATION LAW WITH MULTIPLY DISCONTINUOUS FLUX**

STEFAN DIEHL

ABSTRACT. Flotation is used for recovery of valuable minerals and coals (hydrophobic particles) and in the purification of wastewater. Near the bottom of a flotation column, gas is injected and small bubbles rise through a pulp, which is injected a distance above the gas inlet. The hydrophobic particles of the pulp attach to the bubbles and float to the top of the column, where a third inlet of wash water is located. The hydrophilic particles remain in the water which flows out at the bottom. Flotation can be seen as the separation between air bubbles and a suspension of fine high density particles (gangue). The drift-flux theory [5] is often used to describe the flotation process in steady state, e.g., [1, 3, 4].

In this work, the volume fraction of bubbles is modelled with a 1D scalar hyperbolic conservation law, which contains a nonlinear drift-flux function and three source terms. By utilizing the theory for conservation laws with discontinuous flux function [2], all steady-state solutions of the drift-flux theory are characterized. Numerical simulations yield the transient behaviour between steady states.

This is a joint work with Raimund Bürger and María Carmen Martí, Universidad de Concepción.

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**EFFECT OF SALINITY ON THE DYNAMICS OF FLOCCULATION OF
COPPER SULPHIDE TAILINGS WITH CLAY CONTENT**

CLAUDIA CASTILLO^{†,*} AND CHRISTIAN IHLE^{*}

ABSTRACT. The need to reduce water consumption in mineral processing has driven several Chilean mining companies to consider the use of seawater in their operations. On the other hand, the consistent increase of fine contents in the mineral due to the progressive decrease in ore grades, and in particular in the tailing stream, imposes new operational challenges, particularly in the thickening and disposal operations.

The present research deals with identifying the role of water salinity -both using NaCl in pure water and seawater- on the flocculation efficiency of a copper sulphide tailing including kaolinite, a commonly found clay in Chilean plant feed minerals. An experimental investigation has been made using a set of reactors working at various agitation speeds and measuring chord length distributions (CLD) using a focused beam reflectance measurement system (FBRM). CLD measurements have been combined with conventional settling tests.

Results show that at fixed flocculant dosing, typical of industrial thickener operation, there is a significant influence of salinity. Given the aforementioned agitation system, a set of optimum values of the mean shear rate has been found. This reflects the relevance of having flexible feedwell mixing conditions in the equipment, and even suggests alternative process paths for water reclamation systems. The present work also exposes the considerably high sensitivity of results with CLD post-processing, an aspect that is discussed in light of derived research lines related to computational processing of laboratory test data.

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**CFD SIMULATION OF CATION EXCHANGE IN SLURRY PIPELINE
FLOW**

CRISTIAN REYES AND CHRISTIAN IHLE

ABSTRACT. Slurry pipelines transporting a coarse and a fine fraction (often related to the presence of clays), both in the presence of seawater, can cause an alteration of the liquid phase chemical composition. In the present paper, to expose the contributions of the coarse and the fine phase on the overall ion exchange problem we present the result of a set of two-dimensional numerical simulations using a mixture model.

The continuity and momentum equation for both the coarse and fine phase, coupled with a model for the transfer of three ionic species (Ca^{2+} , Na^+ and Mg^{2+}) has been implemented using the OpenFOAM library. The flow is assumed turbulent, and to this purpose, the k - ϵ model has been used. The mass transport has been modelled using a two-species first order kinetic model derived from the Gaines-Thomas exchange equation, assuming a relation between the rate of Ca^{2+} - Na^+ and Na^{+2} - Mg^{+2} exchange.

Results reveal the presence of an inhomogeneous concentration distribution in the vertical and the fine fraction vertical mobility *via* settling. This is related to variable local residence times, promoting higher Ca^{2+} - Na^+ exchange rates near the bottom than in the axis of the pipe within the column. The potential for future directions of this research is discussed in light of present results.

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**FULL SCALE MEASUREMENTS AND MODEL DEVELOPMENT FOR
REACTIVE SETTLING OF ACTIVATED SLUDGE**

ELENA TORFS

ABSTRACT. Most models of the settling processes in wastewater treatment plants (WWTPs) are based on the assumption that only physical separation is occurring in the settling tanks and that there are no biological reactions taking place [1]. However, at long residence times and incomplete denitrification in the upstream bioreactor, a significant amount of denitrification can take place at the bottom of the tank, where the concentration of sludge is high, nitrate levels are substantial, biomass decay kicks, and no oxygen is present [2]. Hence, mathematical models that are able to capture the mechanical sedimentation-compression process in a SST in combination with biological reactions, in particular denitrification, are needed to allow for the simulation of such operational scenarios.

To study the importance of biological reactions in the settler, an intensive measurement campaign was conducted in a pilot scale wastewater treatment plant (16m³) at Laval university (Canada). Biological conversion processes such as denitrification and decay were monitored in the secondary settling tank under different conditions of sludge blanket height, residence time, nitrate loading and readily biodegradable COD addition. Based on the results of this campaign a thorough discussion will be presented on the impact of reactive settlers in WWTP operation and the ability or limitations of existing models to accurately simulate these conditions.

This contribution is a continuation of recent joint work [3] with Raimund Bürger, Julio Careaga and Camilo Mejías (Universidad de Concepción, Chile), Stefan Diehl (Lund University, Sweden), Ingmar Nopens (Ghent University, Belgium) and Peter A. Vanrolleghem (Université Laval, Canada).

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**GRANULAR PARTIAL NITRITATION/ANAMMOX PROCESS: WHY
MODELING AND MAIN CHALLENGES**

ELISA GIUSTINIANOVICH[†], JOSÉ-LUIS CAMPOS^{*}, CAMILO MEJÍAS[‡],
AND MARLENE ROECKEL[†]

ABSTRACT. Partial nitrification/Anammox process is a novel technology for the complete nitrogen removal from wastewaters, being the most applied at full scale for its technical and economic advantages [1, 2]. It is mainly applied to digester supernatants [3]; but its application on industry effluents is limited by high chemical oxygen demand (COD)/N ratios, which promote the competition between microbial communities [4–7] worsening the reactor performance. Operational parameters as hydraulic retention time and aeration mode can be controlled to overcome competition in granular biomass systems [8], but those limits have not already reported. Operational strategies to improve the removal performance have been detected at laboratory scale in order to feed a mathematical model under development. The process model considers both: reactor and granular scales, which means a global mass balance for the reactor, diffusion/advection/reaction phenomena occurring at the granules and liquid bulk, and growth/detachment processes that determine the granules size. In this work, the model potentials and the main challenges from the mathematical point of view are discussed.

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**Mathematical Modelling for Bioprocesses,
Wastewater Treatment and Mineral Processing
Third CI²MA Workshop, organized jointly with CRHIAM
Universidad de Concepción, September 27 and 28, 2017**

**MODELLING BIOFILM GROWTH IN A
GRANULAR SLUDGE BIOREACTOR**

CAMILO MEJÍAS

ABSTRACT. Between 1980 and 2000 many mathematical models were developed to understand the partial nitrification processes occurring in biofilms that grow as small granules in a reactor, which is fed with dissolved nutrients. Classical works began with [4] and were reviewed in [1]. The contributions [2, 5] form the basis of the widely used software AQUASIM. In the recent thesis [3], Vangsgaard presented new modelling ingredients, whereas some idealized assumptions for critical processes made earlier remained. Although ingredients for a three-phase-flow model can be found in the literature [2], no simulation model seems to have been developed. In the present work, we derive a three-phase-flow model containing a moving-boundary formulation for the system of PDEs modelling the biofilm, suspended particles and dissolved substrates. The PDE system is coupled to a system of ODEs for the bioreactor concentrations. A suitable transformation converts the PDE system to advection-diffusion-reaction form, suitable for numerical implementation. Some preliminary examples will be presented.

This is a joint work with Raimund Bürger, Universidad de Concepción, and Stefan Diehl, Lund University, Sweden.

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