CO_2 Capture and Bioconversion to Biogas in an Anaerobic System using an UASB Reactor

Mahmood Alimahmoodi[1] and Catherine Mulligan[2]

Carbon dioxide is the most dominant component of greenhouse gases and its increasing level in the atmosphere has been of growing concern for many years. There have been many methods to reduce carbon dioxide emissions in the form of CO_2 capture and storage through its injection in the underground waters e.g. saline waters or aquifers in which, CO_2 is transferred from one place to another and there is always the risk of CO_2 release to the environment.

In this research, a new method to capture and conversion of carbon dioxide in an anaerobic system with an UASB reactor (1 L working volume) at 35°C is developed. Acetic acid and mixed VFAs were tested as sources of hydrogen. The system performance was evaluated based on CO_2 and COD removals. Values of 68.7%-85.78% were obtained for CO_2 removal and the overall efficiency values were above 50% for loading rates up to 25 g COD/L.d with high methane contents (>70%) in the biogas.

Also, in a set of batch experiments, the kinetic parameters were obtained using experimental data and a numerical method that was developed in this study to solve the differential equations for substrate utilization and biomass growth.
The method can be applied to reduce CO_2 emitted to the atmosphere from a wide variety of industrial point sources with a value added product, methane.

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Equilibrium Phase Partitioning and Bioavailability of Petroleum Hydrocarbon-Contaminated Soils at Low Temperatures and under Freeze-Thaw Cycles

Maha Zaabri[1] and Subhasis Ghoshal[2]

Substantial soil contamination has occurred in cold, northern regions as a result of oil spills. Traditionally, bioremediation was assumed to come to a halt during the winter season, but today various investigators have reported that biodegradation of oil components in soil can in fact occur at these low temperatures (-5 to 7 ^{o}C) and at rates that are comparable to those present at ambient temperatures. More recent investigations have concluded that the bioavailability of hydrocarbons may be increased by freeze/thaw cycles, but the reasons behind the increased bioavailability have not been explained.

The effects of low temperatures on equilibrium-phase partitioning and aqueous solubility, parameters that affect the rate of bioremediation, are not fully understood and thus knowledge on phenomena that limit the rates and extent of biodegradation is lacking. This research focuses on studying, through calculations, and through experiments using batch and column systems, how cold temperatures in soil and soil-free systems affect relevant physicochemical processes. Particularly, the effects of low temperatures on equilibrium phase partitioning will be evaluated.

Prediction models for bioremediation in cold regions require knowledge of the physical-chemical properties of the contaminants at low temperatures. A review of previously developed equations that express the dependence of vapour pressure and solubility on temperature is presented. This allowed for a comparison of the equilibrium partitioning of naphthalene from dodecane and crude oil at different temperatures (8^{o}C and 25^{o}C). The research results are important for sub soils and ground waters of regions like Quebec where low temperatures predominate.

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Effect of Naphthoquinone, Dihydroxynaphthalene, and Siderophore on Biodegradation of Naphthalene and Reduction of Hexavalent Chromium

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Simultaneous decontamination of polycyclic aromatic hydrocarbons (PAHs) and heavy metals by bacteria have been observed and proved to be viable numerous times. In past researches, 1, 2-naphthoquinones were detected during mineralization of naphthalene, and chemically adding the quinone in biodegradation experiments resulted in a significant boost in the naphthalene biodegradation rates, as well as the rate of reduction of chromium. However the mechanism behind this phenomenon remains largely obscure. Laboratory experiments were conducted to verify the suspected mechanism that the quinone had on the system as well as to assess whether the same phenomenon can be observed. The rate of reduction of Cr (VI) with the addition of 1, 2-naphthoquinone by *Pseudomonas putida* ATCC 17484 was observed. Replicating Alaa's experiment, the fast rate of reduction cannot be reached. 1,2-dihydroxynaphthalene was produced when 1,2-naphthoquinone was reduced by chemically added NADH. When 1,2-dihydroxynaphthalene is chemically added to Cr (VI), there is a rapid reduction reaction occurring. It is believed that this chemical is responsible for the observed increase in rate of chromium (VI) reduction. The addition of the siderophore desferrioxamine B, an iron chelating agent, resulted in an instantaneous binding to chromium (VI), thus reducing the toxicity inside the system and increasing the rate of reduction. Furthermore it has been observed that the chelated complex remains stable for a period of 4 days even when subjected to extreme conditions (acid). Mineralization of naphthalene were also monitored when 1,2-dihydroxynaphthalene, and DFB were added respectively.

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Kinetics of Laccase-Catalyzed Transformation of Aqueous Phenol

Selvia Kurniawati[1] and James A. Nicell[2]

Laccase (EC 1.10.3.2) from fungi *Trametes versicolor* catalyzes transformation of phenol in the presence of oxygen. This process has demonstrated a good potential as a method for the removal of phenol and other toxic contaminants from wastewaters. Fully transient and pseudo-steady state models of this system have been developed to facilitate a better understanding of the mechanisms of enzyme-catalyzed transformation and to assist in the choice and design of a suitable reactor system. Model validation was carried out by comparing model predictions with experimental observations of the phenol transformation and oxygen consumption. Good agreement was found between experimental data and predictions of the fully transient and pseudo-steady state models. In the pseudo-steady state model, the assumption of steady-state distribution of the enzyme has been verified and showed an advantage of reduced complexity with a corresponding reduction in computation time required to solve model equations while maintaining the predictive ability of the fully transient model.

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BPA Conversion Catalyzed by Laccase in a Reverse Micelle System

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The catalytic oxidation of bisphenol A [BPA: 2, 2-bis (4-hydroxyphenyl) propane] by laccase has attracted considerable attention due to its potential for effectively transforming toxic contaminants at high rates. The drawback of BPA conversion catalyzed by laccase in the aqueous phase is that the quantity of laccase that is required can represent a significant portion of treatment costs. A study is being conducted in order to see if enzyme treatment costs could be reduced by first extracting the aromatic compounds into a non-aqueous phase where aromatic compounds are substantially soluble. Since laccase does not exhibit significant catalytic activity in organic media, the use of reversed micelles (RMs) has been introduced to enhance laccase activity by providing an aqueous environment for the enzyme. In this work, the oxidation of BPA catalyzed by laccase hosted in a reversed micelle system was investigated. The RMs were formulated with a surfactant, sodium bis (2-ethylhexyl) sulphosuccinate (AOT), and an organic solvent, isooctane. To optimize the reaction conditions, the effects of pH of the RMs, the concentrations of laccase and surfactant in isooctane, and the mass ratio of [H_2O] to [surfactant] (Wo) in RMs were examined. Laccase entrapped in RMs exhibits the highest catalytic activity under the following conditions: pH = 6.0, Wo = 10, [laccase] = 50 μg/L, and [AOT] = 200 mM. Finally, the effects of five mediators on the reaction were examined. It has been suggested that these mediators could be used to accomplish the oxidation of compounds that are not effective substrates of laccase enzyme. The mediator 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid)(ABTS) was found to be able to significantly improve the efficiency of BPA oxidation.

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Assessing Disinfection Efficiency of Combined UV and PAA for a Physicochemical Wastewater.

Shockley Dong[1] and Ronald Gehr[2]

Ultraviolet radiation (UV) is well known as an effective disinfection process for wastewater treatment. One of the drawbacks is the long tailing that occurs on many response-dose graphs. Such tailing implies that there will always be a significant number of surviving bacteria, no matter the value of the UV fluence. This is especially acute with physicochemical effluents with relatively high concentrations of particles. In some cases, then, UV alone may not be able to satisfy target effluent microbial levels. Peracetic acid (PAA) has also been found to be an effective chemical disinfectant for wastewaters, but doses (especially for physicochemical effluents) have been found to be uneconomical.

Recent studies in Italy have determined that the combination of PAA and UV could yield synergistic effects. This synergism was attributed to the production of hydroxyl radicals ($OH^{\bullet}$), a well-known effect which occurs with UV, PAA, and hydrogen peroxide (H_2O_2), which itself is a component of any PAA solution. Hence experiments in the present study were designed to assess whether the combined PAA-UV process could be used to achieve target fecal coliform (FC) levels below 900 CFU/100 mL, at realistic doses, for the physicochemical effluent from the Montreal Wastewater Treatment Plant.

Effluent samples from the primary settling basins (following coagulation with ferric chloride) were tested in batch experiments with PAA alone, UV alone, and a combination of PAA plus UV. PAA doses were 1 mg/L, 2 mg/L, and 4 mg/L at a contact time of 30 minutes. The UV fluences were 10 mJ/cm^2, 20 mJ/cm^2, and 40 mJ/cm^2. In the combination experiments, UV radiation was applied immediately following the addition of PAA in order to facilitate the formation of $OH^{\bullet}$.

The combined PAA and UV tests showed at least an additive effect. Although PAA alone could attain up to 4-log reductions at the highest dose of 4 mg/L, and UV alone could achieve close to this value at 40 mJ/cm^2, in most cases these levels of disinfection could not be attained, and the combination always performed better, in one case reaching over 5-log removals. Furthermore, the target fecal coliform level could in some tests be reached at PAA&UV levels of 2 mg/L&10 mJ/cm^2, and almost always at 2 mg/L&20 mJ/cm^2, and these may indeed be economically feasible levels. Hence this combined process shows great promise for disinfecting "recalcitrant" wastewaters.

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Electrochemical Water Disinfection Using Pulsed Electric Fields

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In recent years, much research in the field of water disinfection has been focused on efficient and cost effective alternatives to chlorine use due to toxic by-products of chlorination. For wastewater treatment, alternatives to expensive chemicals and large treatment plants are also being investigated.

In the liquid food industry, electrochemical treatment using pulsed electric fields (PEF) has produced excellent disinfection results. The use of PEF for water disinfection is a promising alternative to chlorine that has not been extensively studied. Furthermore, water treatment using PEF would create no unwanted by-products, require no addition of chemicals, require relatively little space, and be environmentally friendly.

Disinfection using PEF relies on electrical, physical and chemical mechanisms that take place in the reactor when a voltage is applied between two electrodes. The de-activation of cellular organisms is believed to be caused by the effects of the electric field on cell membranes. What is more, under specific conditions, UV light and shockwaves are produced in the reactor, also having a significant effect on cell de-activation. Oxidative attack by compounds and radicals formed during PEF are thought to be the dominant chemical mechanisms. Oxidation of cells by ozone and OH• radicals play an important role in cell de-activation.

The effectiveness of PEF also depends on the type and number of pulses applied, the nature of the organism of interest (i.e. cell morphology, growth stage, cell size, and number), and the nature of the medium (i.e. conductivity, SS, salinity, oxygen content, temperature and pH).

The objectives of the research are to determine which mechanisms are responsible for the de-activation of cells during PEF water disinfection. In addition, the development of kinetic models is necessary in order to determine the rate and predict the fate of reactions. Finally, different electrode materials and reactor designs will be tested.

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Three-Dimensional Investigations of Recirculating Flow in an Open Channel Embayment with Particle Tracking Velocimetry and Computational Fluid Dynamics

By: Elizabeth Jamieson[1] and Susan Gaskin[2]

In order to better understand the exchange and transport of mass in rivers a new experimental method of quantifying three-dimensional flow structures in open channel flows is presented. It is recognized that the dynamic and often turbulent behaviour of open channel flows control how materials and matter such as sediments, pollutants and nutrients are dispersed and deposited in the surrounding environment. However, the influence of secondary velocities and other three-dimensional effects are of particular interest. The objective of this research is to provide detailed three-dimensional descriptions of the fluid mechanics in recirculating open channel flows using two methods: Particle Tracking Velocimetry (PTV) and Computational Fluid Dynamics (CFD).

Recirculating flows, which occur when flow in the main channel separates (in the case of harbours, bays, embayments or groyne fields) and a circulation pattern or "dead zone" develops, promote low velocities and turbulence within this region, affecting the exchange and transport of mass by increasing deposition and retention time. A three-dimensional PTV technique is used to describe the motion of neutrally buoyant particles, to provide details of the instantaneous structure of the flow field and the dynamics of the large and small scale eddies. In this technique, the flow in a laboratory flume with a square embayment is seeded with phosphorescent particles that are excited by a focused source of UV light and with time sequenced photographs their images (in the plan and profile views) are recorded and processed to obtain 3D quantitative velocity information.

In addition to the experimental study, the CFD code Fluent was used to simulate the three dimensional flow fields and results then compared to the PTV investigation. This software is able to calculate a detailed three-dimensional velocity field to illustrate where secondary velocities are strongest and weakest, and how they relate to the mass exchange and retention time.

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Three-Dimensional Simulation of Flow Past A Slot In A Rectangular Conduit

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The three-dimensional two-equation k-ω turbulence model is applied to obtain the characteristics of flow past a slot located in a rectangular closed conduit. The predictions of the numerical simulation are validated using previous experimental data. The model faithfully reproduces the flow behaviour including flow separation in the expanding flow region downstream of the slot. In particular, the model predictions agree well with the experimental data related to pressure and velocity fields. For other slot flow situations encountered in engineering practice, following model validation, the numerical model yields design data pertaining to flow characteristics for different discharge ratios and slot width ratios.

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Modeling of Transport in a Porous Medium

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The process of transport of a contaminant in a porous medium is an important topic in the geoenvironmental field, and usually involves complication by several nonlinear processes which can range from dissolution of the solid material to the reaction of the chemical or contaminant with the porous skeleton. For such nonlinear problems, experimental work is necessary to test the validity of the theory and to identify the bounds of accuracy of numerical simulation of the processes involved. Also, experimental results can be used to identify the parameters in the model and to reveal nonlinear phenomena in the transport process. This paper examines the transport of dyed water within a column of glass beads for the cases where the boundary flow potential is time-dependent. The transient transport phenomenon of dyed water in the column of glass beads is recorded using digital camera and quantitative values of dye concentration distribution along the column is obtained by the image processing technique applied to digital image. With these experimental results together with an analytical solution, a hydrodynamic dispersion coefficient can be identified and the numerical accuracy of certain stabilized numerical methods can be examined. Experimental facilities can be also used to examine the transport phenomena in an inhomogeneous region consisting of porous media with different porosity.

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An Integrated Zonal Model to Predict Transient Indoor Humidity Distribution

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To investigate the impact of building material moisture adsorption and desorption on indoor air humidity and predict humidity distribution in a room, a zonal model was integrated with building material moisture transfer model. This integrated zonal model was developed based on the conservation of air mass, energy and water vapor mass. The model was applied to a room with forced or natural convection airflow: the model could predict humidity and temperature distribution in the room and shows the influence of building material moisture adsorption and desorption on this behavior. It was found that moisture adsorption and desorption by building materials not only influenced humidity distribution within the room but also affected the moisture content in the building materials. The predictions of the integrated zonal model were compared with the available data in the literature. The results showed that the integrated zonal model, with quite coarse mesh, could provide sufficiently reliable information about airflow pattern, thermal and indoor humidity distributions within a room. The model could be used to analyze building material moisture adsorption and desorption behaviors and provide useful information on the cooling load.

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Three-Dimensional Numerical Modelling of Flow and Sediment Transport During a Controlled Flood in a River

A.O. George[1], P.M. Biron[2] and A.S. Ramamurthy[1]

Controlled floods are often used in rivers to remove fine sediments that accumulate within the gravel particles and which have a negative impact on the survival rate of fish eggs in the substrate. In order to determine whether a given discharge can create sufficient sediment transport to remove the sand particles, accurate estimates of bed shear stress are required. Three-dimensional numerical models can predict in a very detailed way the flow field and bed shear stress very close to the bed. The objective of this study is to use a three-dimensional model to predict near-bed flow field and shear stress during a controlled flood in a natural river. Based on the shear stress distribution, bedload transport rates will be estimated and compared with field measurements. The study site is the Escoumins River (Quebec), where a dam upstream of the studied reach has been used to create control floods. Field measurements on flow and bedload transport are available for this site. Two-dimensional simulations of this reach are also available (model Hydrosim), allowing a comparison between the 3D and 2D approaches. The 3D model used is Phoenics, which solves the three-dimensional form of the Reynolds-averaged Navier-Stokes equations for a steady-state flow (the flood is maintained at the same level for several hours and thus steady-state flow can be used). A body-fitted coordinate grid was generated using the software GEOGRID. Results show that the simulations are strongly affected by the mesh design, particularly in the shallow zones. However, because these zones have lower bed shear stress, it is still possible to calculate relatively accurately bedload transport rates in most of the simulated reach.

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Visualisation and Quantification of Residual Non-Aqueous Phase Liquids in Porous Media using X-Ray Computed Tomography

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Non-aqueous phase liquids (NAPLs), if spilled into the subsurface, will migrate downward, and a significant fraction will become "trapped" in the soil matrix. These "trapped" NAPL globules will partition into the water and/or vapour phase, and serve as continuing sources of contamination (e.g. source zones). At present, the presence of NAPL in the subsurface is typically inferred from chemical analysis data. There are no accepted methodologies or protocols available for the direct characterisation of NAPLs in the subsurface. Proven and cost-effective methodologies are needed to allow effective implementation of remediation technologies at NAPL contaminated sites. X-ray Computed Tomography (CT) has the potential to non-destructively quantify NAPL mass and distribution in soil cores due to this technology's ability to detect small atomic density differences of solid, liquid, gas, and NAPL phases present in a representative volume element. The authors have demonstrated that selected environmentally significant NAPLs, such as gasoline and other oil products, chlorinated solvents, and PCBs possess a characteristic and predictable X-ray CT attenuation number that permits their quantification in porous media at incident beam energies, typical of medical and industrial X-ray CT scanners. As part of this study, methodologies were developed and refined for generating and analysing X-ray CT data for the study of NAPLs in natural porous media. Extracting quantitative information from X-ray CT images requires specialised user-defined functions not available in typical visualisation software designed for medical diagnostic purposes. Additionally, image data requires pre-processing such as filtering, normalisation to remove drift, post-scan calibration/correction, truncation of excess data, and centring of study object within data array. A series of MATLAB programs were developed by the authors specifically for pre-processing and analysis of non-medical x-ray CT data. The computational methodology entails image subtraction in order to isolate and quantify the phases of interest (i.e. air, water, NAPL) Columns of NAPL-contaminated soils were scanned, flushed with solvents and water to remove entrapped NAPL, and re-scanned. X-ray CT data was analysed to obtain numerical arrays of soil porosity, NAPL saturation, and NAPL volume at a spatial resolution of 1 mm. This methodology was validated using homogeneous and heterogeneous sands soil columns with known quantities of gasoline and tetrachloroethylene. NAPL volumes computed using X-ray CT data was compared with known volumes from volume balance calculations. Error analysis revealed that the NAPL measurement technique is subject to a 6% error mainly due to instrument noise and column positioning errors. Residual NAPL saturation in soil cores averaged 10% and varied spatially from less than 1% to 70%. These results and others serve as proof that a typical medical X-ray CT scanner has the potential to accurately quantify, in three-dimension and at small (1mm) spatial resolution), selected NAPLs in natural soils.

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Water Demand Management in the Caribbean: A Case Study of Barbados

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The management of our water resources has predominately focused on augmenting supplies to meet the demands for water. However, less attention has been given to the sustainable, efficient and equitable use of water. It is now recognized that more emphasis should be placed on managing water from a demand side. Water demand management can be used to raise water use efficiency, improve social equity and development, and sustain water supply and services.

Water demand management (WDM) is necessary in water scarce regions like Barbados, which is ranked among the world's ten most water scarce countries. This Caribbean island is almost entirely dependent on groundwater to meet the various water demands. The Government of Barbados has recognized the need for WDM as demonstrated by the implementation of measures such as universal metering, water pricing, reduction of unaccounted for water, and public education campaigns.

This research evaluates the impact of various variables affecting residential water use in Barbados such as metering, water pricing and income. An understanding of the effects of these variables is crucial to analyze the impacts of future water demand management policies such as increasing water tariffs.

To asses the potential of price and metering as tools to conserve water demand in Barbados, an econometric demand model of residential water demand has been developed. The analysis relies on cross-sectional annual time-series data for seven districts in the parish of St-James, Barbados. Residential demand is estimated as a function of income, water price and rainfall. Elasticities for these three variables are calculated. The results compare well with past residential water demand studies and confirm the hypothesis that water price does have a positive effect in reducing domestic water demands. Furthermore, preliminary results indicate that water production decreased considerably from 1997 to 2000, coinciding with the implementation of the Universal Metering Program.

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GIS as a Tool to Improve Water Management

Jaime Carrera[1] and Susan Gaskin[2]

The concept of water management evolved from a piece meal approach to a Basin level management after the International Conference on Water and Environment in 1992. This concept shifted to Integrated Water Management in Rio later that year. Behind this idea was the introduction of land and water related aspects in water management at the Basin level. However, this seldom occurs in practice, mainly due to a lack of proper tools to achieve an integrated river basin and sustainable approach. These tools should help to simulate, visualize and compare different water management scenarios. Data must be accessible to all interested stake holders; this accessibility can be provided by the use of Relational Database Management Systems (RDBMs) which can integrate both quantitative and qualitative data. The use of a GIS will help to visualize and update the existing database. Superimposition of different layers can be done in order to verify existing data; also the existing modules of a GIS can be used to analyze the data (e.g., basic statistics, buffer analysis and geostatistics). In order to illustrate the proposed approach, the Basin of Mexico will be used, as it encloses one of the biggest cities in the world: Mexico City and its Metropolitan Area (MCMA).

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An Experimental Study on a Fish Louver System

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Fish populations are dropping drastically in many rivers in North America where hydropower dams have been erected. The fish are either blocked from passing or damaged when migrating downstream past dams. Several solutions have been suggested to help mitigate this problem. Fish screens have been installed at canal and turbine intakes to block the fish from reaching the turbines and spillway. A bypass is placed next to these screens to provide an alternative route around the dam or any hydraulic installation.

Another mitigation measure is to use "Fish Louvers" which guide the fish towards a bypass around the dam. This paper provides an overview concerning the history and use of fish screens, and the development of fish louvers and their application in two case studies.

An experimental study was conducted on a partial physical scale model of fish louvers. The objective of this study was to determine the head losses generated when the fish louvers are installed upstream of a power canal. The model was run under different scenarios in which the channel flow and bypass flow where varied. Three prototype channel flows were tested: Q=3100, 5100, 7100 cfs, with four prototype bypass flows: bypass closed, Qbypass=0, 200, 350 cfs. The head losses were measured using two manometers located upstream and downstream of the louver rack. Maximum head losses reaching 2 ft (prototype) where recorded when the bypass was closed. These head losses dropped by half when the bypass was opened. The upstream velocities on the face of the louver racks were measured with a propellor meter to verify if they were below the threshold which the fish can sustain before being pushed through the louver vanes. Results have shown that the upstream velocities in all but one case were less than 7 fps and consequently are sustainable by the fish. The velocities increased with increasing the channel and bypass flows.

Further research needs to be conducted, that will include varying more parameters, in order to minimize generated head losses. Floating louvers and flow straighteners are two ways of optimizing their performance. Studying the effects of changing the louvers spacing and the vanes' thickness would be highly rewarding.

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A Systematic Assessment of Global Optimization Methods for Conceptual Hydrologic Models Calibration

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The major difficulty concerning the use of conceptual rainfall-runoff (CRR) models in practice is related to their calibration since most of these models involve a large number of parameters. In general, the CRR model calibration could be considered as a global optimization problem since its main objective is to find a set of physically plausible model parameter values such that the best fit between observed and estimated flow hydrographs could be achieved. Hence, several global optimization methods (GOM) have been proposed in hydrology. However, there is no general agreement as to which method is the most appropriate one for CRR calibration purposes. The main objective of the present paper is therefore to propose a systematic procedure for assessing the performance of various GOM methods based on their robustness, accuracy and efficiency in the calibration of CRR models. More specifically, the proposed procedure consists of evaluating systematically seven popular methods: the Multistart procedure based on the simplex local optimization technique (Nelder, 1965), the Control Random Search (CRS) method (Price, 1983), the original Shuffled Complex Evolution (SCE) method (Duan et al., 1993), the Simulated Annealing (SA) method, the Tabu technique (Chelouah and Siarry, 1998), the Cluster method (Solomatine, 1995), and the modified SCE method using the grid concept as suggested by Muttil and Liong (2003). In the present study, the performance of these different calibration methods were judged based on the use of a number of traditional benchmark theoretical functions with known global optima as well as relying on the rainfall-runoff simulation given by a typical TANK model for both cases of real and synthetic streamflow data. Results have indicated that the Multistart and the original SCE methods are the most accurate and robust while the CRS and Cluster methods are the most efficient. The SA and Tabu techniques were found to be the least satisfactory. Results have also pointed out the limitation of the modified SCE method. Finally, it has been observed that it is still difficult to take explicitly into account the interactions between model parameters using existing calibration procedures.

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