Seventh Brace Research Day – February 14 2008
List of Presenters and times

9:25 **Keynote Speaker:** Professor A.P.S. Selvadurai: Advective Transport in Porous Media: Analytical, Computational and Experimental Approaches. *Civil Engineering and Applied Mechanics page 2*

10:10 Coastal Erosion by Waves. Lai Wai Tan, *Civil Engineering and Applied Mechanics page 3*

10:30 Environmental Prediction in Canadian Cities: Measuring Montreal and Vancouver's Urban Energy Balance. Eric Christensen, *Natural Resource Sciences page 4*

11:00 Studying Bacterial Growth Environmental Biotechnology: How to Use Genomic Data. Mohammad Tajparast, *Civil Engineering and Applied Mechanics page 5*

11:20 Examining the Importance of Oxygen Tension on Bacterial Adhesion and Migration in Artificial Groundwaters. Felipe Castro, *Chemical Engineering page 6*

11:40 From Forest to Lake: An overview of the Effect of Hydroelectric Reservoir Impoundment on CO2 Fluxes. Marie-Ève Lemieux, *Natural Resource Sciences page 7*

13:00 Plant Water Status and Soil Moisture Condition as Indicators of Irrigation Needs of Peaches and Grapes in Southern Ontario. Rufa Doria, *Bioresource Engineering page 8*

13:30 Removal of Veterinary Antibiotics by a Constructed Wetland. Azfar Hussain, *Bioresource Engineering page 9*

13:50 Evaluation of On-farm Irrigation to Improve Water Use Efficiency. Marie-Hélène Bernier, *Bioresource Engineering page 10*

14:10 Reuse of Domestic Greywater for Irrigation of Food Crops. Sara Finley, *Bioresource Engineering page 11*

14:30 A Quartz Crystal Microbalance Based Biosensor for Detection of Pathogenic Bacteria in Water. Charles Poitras, *Chemical Engineering page 12*

15:05 Nitrate and Orthophosphate Reduction from Agricultural Runoff in a Surface-Flow Constructed Wetland. Charlotte Yates, *Bioresource Engineering page 13*

15:25 Optimizing Drain Water Reuse in Greenhouses. Moshe Halpern, *Natural Resource Sciences page 14*

15:45 Predicting Concentrations of Micropollutants along the Wastewater Treatment and Collection Train: Making a Case for Source Separation. Usman Khan, *Civil Engineering and Applied Mechanics page 15*

16:05 Water and Nitrogen Use Efficiency of Corn under Different Water Table Management Condition. Ajay Singh, *Bioresource Engineering page 16*

16:25 Estimation of Design Storms in Consideration of Climate Variability and Change. Nicolas Desramaut, *Civil Engineering and Applied Mechanics page 17*

ADVECTIVE TRANSPORT IN POROUS MEDIA: Analytical, Computational and Experimental Approaches

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ABSTRACT

The transport of chemicals and other contaminants in porous geological media is a topic of fundamental importance in the general area of geosciences and of particular interest to geo-environmental engineering. The basic mechanisms of transport range from advective transport, which depends on an advective flow velocity, to diffusive transport that depends on a concentration gradient. Although the fundamental processes governing these basic modes of transport can be highly non-linear and dependent on the micro-structural morphology and chemistry of the contaminant and the porous medium, the linear theories associated with these basic transport processes provide useful first approximations for the study of both advective and diffusive processes. The advective process in particular provides estimates for the time and spatial distribution of the chemical species in the porous medium which constitutes an important input to the environmental decision making process. The methodologies available for the solution of the classical advective transport equation has evolved over the past three decades and these approaches can vary from purely analytical techniques to several computational schemes that tend to minimize numerical errors associated with the solution procedure. This lecture will focus on the calibration of the advective transport equation associated with time-dependent advective velocities. The time-dependency in the advective velocities can be a result of time-dependent variations in the boundary flux associated with the potential problem. The calibration of the computational procedure for the linear advective transport with time-dependent velocities is facilitated through recently developed analytical solutions for multi-dimensional advective transport problems. The robustness of the numerical schemes are particularly challenged when the chemical migration profiles have a *discontinuous front* and the advantages of diffusive phenomena are not available to mitigate processes such as overshoot and negative values in the chemical concentration profile. The lecture presents the overall calibration of the computational approaches with analytical results and uses the methodologies to examine the advective transport in a one-dimensional experimental configuration involving time-dependent advective flow velocities.

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Coastal erosion by Waves

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Sea level rise change the delicate balance between erosion and accretion. The study of the erosion has become a topical problem recently with increase interest in adaptation to climate change. Numerous numerical models have been developed to study wave erosion problem. However, most are not reliable. The main obstacle to progress is numerical instability. The difficulty is at the wave front, where the water meets the erodible bed. Numerical oscillations can lead to negative water depth and subsequent collapse of the numerical computations. Shock-capturing methods have been developed to control the spurious oscillations due to rapid change of water depth at the wave front. An artificial wet bed is required even with the shock-capturing scheme. These difficulties have prevented accurate simulations of the wave front in an area where erosion and accretion is often the dominant process. The purpose of this paper is to introduce a robust computational method, referred to as the Lagrangian Block on Eulerian Mesh (LBEM), for the simulation of waves on erodible bed. Simulation of waves by LBEM is compared to a more conventional finite volume method. LBEM simulations results have been compared to analytical solutions for model verification. Currently, the LBEM is being validated on the sediment transport problem. It is also being extended to a two-dimensional model for general simulation of coastal erosion over arbitrary topographies. The ultimate goal is to employ the robust LBEM to mitigate problems such as wave overtopping levee, flooding due to storm surges, and to reduce damages by tsunami.

Environmental Prediction in Canadian Cities: Measuring Montreal and Vancouver's Urban Energy Balance.

Eric Christensen and Ian Strachan
Dept of Natural Resource Sciences

The urban heat island is a phenomenon involving the consistent occurrence of warmer temperatures within cities relative to the surrounding countryside for a given period. This stems from the unique geometry of urban environments, the darker surfaces composing the city fabric, the limited availability of water and the direct input of heat by human activities. These characteristics engender the heat island by altering the surface energy budget. At the same time, they complicate weather forecasting techniques through our incomplete understanding of exchange processes related to urbanization. With over 80% of Canada's population now living in cities, it is important to understand and be able to model the urban energy balance in order to deliver precise and exact weather predictions. The Environmental Prediction in Canadian Cities (EPiCC) network operates under the mandate of collecting high precision time resolved energy flux data from select sites in Vancouver and Montreal with the objective of comparing it to numerical models specifically parameterised for those cities. The ultimate goal is to couple the city scale simulation of the energy budget with larger scale models in order to include important feedback relationships. This presentation focuses on how the urban surface energy budget differs from that of the rural environment and on how the EPiCC project aims to measure these differences and apply them to bettering weather forecasting in Canada.

Studying Bacterial Growth Environmental Biotechnology: How to Use Genomic Data?

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The mathematical modeling to predict and optimize the operation of biological wastewater treatment processes have greatly progressed over the past two decades. In order to build the next generation of models, we now aim at incorporating genomic and metagenomic information to define microbial activities. In this presentation, we will present the general approach to do built what we can a genome-scale metabolic model. Briefly, one first establishes a detailed theoretical framework which lists as many metabolic reactions as possible using genomics data. In a second step, the molecular fluxes through each reaction need to be calculated to determine how the cell functions. To do so, physico-chemical constraints are added to the model to restrict the number of possible solutions. The main constraints are the well defined conservation laws (i.e., conservation of mass, energy and electric charges). Then, Flux Balance Analysis (FBA) can be used to determine the metabolic phenotype (characteristic functioning of the metabolic network) to the genotype in different growth conditions. However, as the number of reactions to consider is usually much greater than the number of metabolites, the systems are often said to be underdetermined and it is impossible to solve the flux balance. In such cases, we need to supplement the analysis with the function that the cell is likely to optimize and find the flux balance solution by of the network of reactions by Linear Programming (LP). Therefore, one needs to determine the proper assumptions to solve the metabolic network. We are currently developing *in silico* genome scale reconstruction of cellular metabolic of the environmentally significant bacteria *Rhodococcus* RHA1, a gram-positive actinomycete known for its superior ability to degrade polychlorinated biphenyls (PCBs) and other aromatic pollutants. By analyzing the growth of *Rhodococcus* RHA1 using the genome-scale metabolic model, we hope to elucidate specific metabolic behaviors of bacteria growing in activated sludge wastewater treatment systems.

Examining the Importance of Oxygen Tension on Bacterial Adhesion and Migration in Artificial Groundwaters

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In Canada alone, nearly 9 million people rely on groundwater as their source of drinking water. The contamination of this potable water supply by microbial pathogens and parasites as a result of infiltration of livestock wastes, leaking septic systems and sewer lines is of significant concern. Although the contamination of groundwater supplies has been linked with outbreaks of disease, the physical, chemical, and biological factors controlling pathogen filtration in the complex subsurface environment are still not well understood. Moreover, many investigations of microbe migration in granular porous matrices have been conducted with nonpathogenic laboratory strains under conditions of little environmental relevance (e.g., nonrepresentative water oxygen tensions). Little is known regarding the transport and retention properties of toxigenic microorganisms, such as E. coli O157:H7, in microaerophilic environments such as those commonly observed in the natural subsurface.

Bacterial cell surface properties are recognized as the key factors that influence bacterial adhesion to surfaces. Among the critical surface properties are surface hydrophobicity, extracellular polymers, and surface electrostatic charge. In the natural subsurface, varied dissolved oxygen (DO) concentrations may be found and little is known about the influence of this factor on the transport and removal of pathogenic microorganisms in such environments. In this study, we evaluated the migration behavior of selected relevant pathogenic microorganisms in water saturated granular systems representative of natural subsurface environments. Escherichia coli O157:H7 and Yersinia enterocolitica were selected based on their importance as pathogens of concern in North American watersheds and their prevalence in agricultural settings. Experiments were conducted using laboratory-scale packed columns over extreme DO solution conditions (microaerophilic and saturated at room temperature). Our results illustrate the importance of considering physicochemical conditions relevant to the natural subsurface environment when designing laboratory transport experiments as evidenced by variations in microbe migration when the microorganisms are acclimatized and transported in different DO environments. The observed differences in the transport potential of these pathogens were found to depend strongly on the growth conditions under the tested environmental settings.

From Forest to Lake: An overview of the Effect of Hydroelectric Reservoir Impoundment on CO_2 Fluxes and the Net Ecosystem Exchange

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Although hydroelectricity is generally believed to be an environmentally-safe way to generate power, it has been suggested that artificial reservoirs could constitute an anthropogenic source of greenhouse gases (GHGs). Within Canada, Quebec is the province holding most of the total hydroelectric production. To date, despite a general knowledge that reservoir creation releases GHGs, especially from tropical measurements, no serious study has attempted to quantify GHGs emissions in a boreal environment through a comparison of the carbon exchange within the pre- and post-flooding environments.

On November 5th, 2005, in Eastmain, Northern James Bay, a total area of 604 km2 was flooded for hydroelectricity purposes. Prior to the impoundment, Hydro-Quebec proposed a multidisciplinary research project, which aimed to quantify the aquatic, terrestrial and atmospheric emissions of CH_4 and CO_2, prior to and post flooding.

Through continuous carbon flux data obtained from micrometeorological technique and meteorological instruments, my research aims to answer the following question: ‘What is the magnitude and direction of carbon exchange from a boreal forest ecosystem when flooded for hydroelectric purposes?”

The overall GHGs assessment project will provide the first continuous measurements of carbon exchange from a newly created hydroelectric reservoir within the boreal region. This work will provide data that will be used in modelling efforts to understand the longer term carbon exchange of this modified ecosystem.

Plant Water Status and Soil Moisture Condition as Indicators of Irrigation Needs of Peaches and Grapes in Southern Ontario

Rufa O. Doria and C.A. Madramootoo
Dept of Bioresource Engineering

To obtain accurate and reliable information on when to trigger irrigation of peaches {Prunus persicae} and grapes {Vitis vinifera} in Southern Ontario was the main objective of this study. Plant-based indicators linked to climatic and soil moisture conditions were evaluated for both irrigated and non-irrigated treatments. Sap flow meters by Dynamax were used for in situ determination of plant water consumption, Theta Probes from Delta-T Devices were installed simultaneously to monitor the soil moisture levels at 3 depths (10, 30 and 50 cm), and potential evapotranspiration (ETo) were determined at the same time by calibration using Penman-Monteith equation in a specific field condition. Analyses were done on how the sap flow responded to the root-zone soil water conditions and potential evaporative demand in both irrigated and non-irrigated peaches and grapes. Results showed that both relationships between sap flow and climatic variables such as air temperature, vapor pressure deficit (VPD) and ETo have considerable degree of agreement. Diurnal patterns of sap flow for irrigated treatment showed a steep increase in the morning until it achieved maximum rates at midday when VPD was at its maximum, then gradually deceased until late afternoon, while non-irrigated treatment showed invariably lower daytime sap flow. Volumetric soil water content (SWC) in irrigated treatment constantly recorded between near field capacity (FC) to 70%FC depending on the type of soil. While for the non-irrigated, SWC decreased progressively until wilting point was reached in the month of July. In conclusion, irrigation decisions can be accurately supported by continuous recording of sap flow in conjunction with real-time monitoring of soil moisture conditions.

Removal of veterinary antibiotics by a constructed wetland

Azfar Hussain and Shiv Prasher
Dept of Bioresource Engineering

The presence of low level of human and veterinary pharmaceuticals has been confirmed in environmental waters by numerous studies. The in hand study principally targets the agricultural source of these emerging contaminants and evaluates efficiency of a surface wetland in removing veterinary pharmaceuticals from wastewaters. A constructed wetland with two textural classes of soils (coarse and fine) was used for this study. A comparable vegetation stand was maintained in both soil sections. Monensin, Salinomycin and Narasin ionophore antibiotics were selected for this study. The results generated in the first year of study did not indicate any appreciable removal of pharmaceutical compounds by the surface flow wetland, however relatively more removal was recorded in the coarse soil. For the lower concentration used Monensin was observed to have higher mobility in the wetland (59.1%-73.9%) whereas, relative mobility for Narasin and Salinomycin ranged between 39.7%-60.4% and 40.9%-53.1%, respectively. In the same set-up, sphagnum peat moss was also appraised for its potential to capture pharmaceutical compounds in the wastewater. Peat gave complete removal in the lower concentration range (100 µg L-1); whereas the removal percentage decreased progressively with increasing levels of antibiotics used (1000 µg L-1and 3000 µg L-1). The low removal potential of surface wetlands for pharmaceutical compounds can be greatly enhanced by incorporation of peat as a complementing wetland substrate.

Evaluation of On-Farm Irrigation to Improve Water Use Efficiency

Marie-Hélène Bernier and Chandra Madramootoo
Dept. Bioresource Engineering

In Southern Ontario, high value horticultural production currently faces considerable competition for limited water resources, a condition exacerbated by expansion of the agricultural sector, increasing urban development and tourism, and potential climate change impacts. As such, water conservation strategies for horticulture irrigation have become a high priority. Solutions for this growing challenge include improved irrigation scheduling techniques, soil moisture monitoring, and evaluation of current water consumption patterns.

As part of a broader study on the development of advanced irrigation scheduling technologies in southern Ontario, four field sites were selected to evaluate eight soil moisture monitoring devices. A questionnaire was developed to collect baseline information on the producers' current irrigation scheduling practices and perceived water needs. A second survey was then conducted, at the end of the growing season, to determine producers' satisfaction with the soil moisture monitoring sensors. The collected information obtained with these surveys was then used to assess irrigation performance while at the same time determining how useful the sensors were to improve water use efficiency. According to the surveys' results, the growers who were inadequately meeting the crop water requirements were found to be very receptive to adopt soil moisture monitoring sensors. This illustrates how feasible the implementation of soil moisture monitoring is, how it can help the industry performing water savings and in the end, reduce the vulnerability of the industry to increasing competition and drought frequency.

Reuse of Domestic Greywater for Irrigation of Food Crops

Sarah Finley and Suzelle Barrington
Dept of Bioresource Engineering

This study examines the feasibility of reusing domestic greywater for the purposes of vegetable garden irrigation at the household level. It focuses on the contamination of crops by pathogenic organisms, the primary health concern associated with greywater reuse for edible crop irrigation. Greywater from a family home was collected and analyzed both raw and after treatment by settling and slow sand filtration, over a period of eight weeks. During that time, both greywaters were used to irrigate individually potted triplicate plants of lettuce, carrots and peppers in a greenhouse. Greenhouse tap water was used as a control. Upon maturity, plants were harvested and the edible portions tested for the presence of Fecal Coliforms and Fecal Streptococci, common indicators for the presence of pathogenic organisms. Results showed high levels of indicator bacteria in the greywater, but no significant difference in contamination levels was observed between crops irrigated with tap water, raw and treated greywaters. Contamination levels for all crops were low and do not represent a significant health risk.

A Quartz Crystal Microbalance Based Biosensor for Detection of Pathogenic Bacteria in Water

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Bacteria are pathogens of concern which may be introduced into the natural environment from land disposal of treated wastewaters or animal fecal deposits. To minimize the impact of these pathogens on the environment and public health, accurate procedures are needed to evaluate their presence and concentration. A direct, real-time method for detection and quantification of target organisms would thus be very useful for rapid diagnosis of water safety. A quartz crystal microbalance with dissipation monitoring (QCM-D) based biosensor for detection of waterborne pathogens (i.e., Escherichia coli O157:H7 has been developed. The detection platform is based on the immobilization of affinity purified polyclonal antibodies onto gold coated QCM-D quartz crystals. The antibody is attached to the gold surface via a self-assembled monolayer of cysteamine. Binding of bacteria to the immobilized antibody gives rise to a decrease in the crystal's resonant frequency and an increase in the energy dissipated above the crystal, allowing for detection of pathogens in aqueous media. The following sensor responses have been investigated: frequency and dissipation shifts after 60 minutes of exposure to bacteria and the initial slope of both the frequency and dissipation shifts. The results reveal that the best option for sensor response is the initial dissipation slope. Selectivity of the biosensor has been examined and demonstrated using a Gram positive organism (Bacillus subtilis). Development of the biosensor will be discussed and the performance of the biosensor over a range of bacteria concentrations will be examined.

Nitrate and orthophosphate reduction from agricultural runoff in a surface-flow constructed wetland

Charlotte Yates and Shiv Prasher
Dept of Bioresource Engineering

The application of this surface-flow, constructed treatment wetland is reduction of agricultural non-point source water pollution. The goal of this project is to determine if the substrate type influences the nitrogen and phosphorous reduction capabilities from agricultural runoff water in Southern Quebec.

The pilot-scale constructed wetland site is located 3 km north of McGill's Macdonald campus in the west of Montreal, Canada. The design consists of six open plastic tanks: three replicates of a sandy clay loam soil, and three replicates of a sandy soil. All six open tanks are planted with cattails and reed canary grass. Each tank has a volume of 5.5m3 with 70% occupied by soil and a mean residence time of approximately 2.1 days. From July to September 2007, the tanks were flooded continuously with an artificial runoff wastewater, containing 10mg/L nitrate-N and 0.3mg/L orthophosphate.

Weekly water samples from the outflow of the tanks were collected and analyzed for nitrate-N, orthophosphate and dissolved organic carbon during the three months of operation. Gas samples were collected every two weeks and tested for nitrous oxide as an indicator of denitrification activity. Results show that as the season progressed, the nitrate removal increased. The removal efficiency in the sandy soil tanks averaged 44% at the beginning of July and increased to 70% by the end of August. The sandy clay loam tanks averaged 55% at the beginning of July and increased to 80% by the end of August. The orthophosphate results showed an opposite trend of removal efficiency, i.e. decreasing as the season progressed. We found that there was no difference between the two soil types in orthophosphate removal.

Optimizing Drain Water Reuse in Greenhouses

Moshe Halpern and Joann Whelan
Dept of Natural Resource Sciences

Canadians are well aware of the need to conserve our fresh water reserves. In Ontario, greenhouse producers are switching to a semi-closed irrigation system that recycles the water draining from plant pots. This water is mixed with fresh water and recirculated through the irrigation system for several weeks, then disposed. In this system, NaCl accumulation limits the number of weeks that water can be recirculated. The objective of the study is to develop a mathematical model to predict the NaCl accumulation over time in the recycled water, and to ascertain whether introducing a salt-absorbing halophyte, Portulaca oleracea L. (Common purslane) into the drainage system is a feasible way to reduce NaCl accumulation. The experiment is a factorial complete randomized design with two treatments: the NaCl concentration in the fresh irrigation water (0 mmol/L, 1 mmol/L and 10 mmol/L), and the presence/ absence of purslane in drainage system. There are four replicates for each treatment. The NaCl concentration in the recycled water is to be measured bi-weekly. The data from these measurements will be used to calibrate the mathematical model developed for a greenhouse with potted plants, which is adapted from a published model of NaCl accumulation in the "Nutrient Film" hydroponics system. The data will also be analyzed to determine whether introducing purslane into the drainage system changes the rate and magnitude of NaCl accumulation in recycled water. This presentation focuses on the theoretical basis for the mathematical modeling of NaCl accumulation in recycled water of greenhouses, and proposes an experiment to calibrate and validate model assumptions.

Prediction of micropollutant concentrations along the wastewater collection and treatment train: making a case for source separation.

Usman Khan & Jim Nicell
Dept of Civil Engineering and Applied Mechanics

One of the fastest growing concerns in the wastewater treatment industry is the environmental presence of pharmaceutically active compounds and estrogens. Such compounds are primarily excreted by humans in urine, either in an unchanged form or as metabolites. In the present day treatment context, urine is collected simultaneously with fecal matter and diluted by large amounts of greywater from domestic sources and other sources of aqueous wastes or water infiltration entering sewer systems. This relatively dilute and complex mixture is then transferred to sewage treatment plants for treatment. Ultimately, effluents from sewage treatment plants are the single most important point source of pharmaceuticals and estrogens into the environment. The purpose of the paper will be to present a modelling approach that would allow one to predict concentrations of pharmaceutically active compounds and estrogens along the wastewater collection and treatment train. Namely, the model would allow simultaneous prediction of urine, influent and effluent concentrations of such compounds. The results of the modelling approach will have two major implications:

1. It would allow one to assess where along the wastewater treatment and collection cycle should one treat such compounds
2. Secondly, the modeling approach along with comparative toxicological data would suggest to one which pharmaceutically active compounds and estrogens should be prioritized for detailed environmental risk assessment and extensive environmental monitoring.

Water and Nitrogen Use Efficiencies of Corn under Water Table Management

Ajay K Singh[1], Chandra A Madramootoo[1], Xiaomin Zhou[2] and Donald L. Smith[2]
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Corn is one of the major commercial crops of North America. It's the major source of food for both humans and livestock. Water and nitrogen are two important components that affect the yield of all crops. While there have been numerous studies on water and nitrogen use efficiencies, there is a lack of research which examines water and nitrogen efficiency in different water table scenarios. There is concern about nitrogen leaching from tile drainage systems, thereby affecting the survival of aquatic ecosystems. Water table management has proven to mitigate this risk. Therefore, this study investigates the water and nitrogen use efficiencies of corn under different water table scenarios in both controlled environment (greenhouse) and field conditions.

Lysimeters were constructed in the greenhouse with a water table maintained at 50 cm from the soil surface, and planted with corn. Four nitrogen treatments of 100, 140, 180 and 270 kg/ha were applied to the lysimeters. Stem gauges were connected to the plant stems in order to measure sap flow. This data enabled an estimation of both water uptake by the plants and evapotranspiration. A portable photosynthesis system LI -6400 was used to measure the photosynthesis. The study was repeated at a field site in Bedford, QC. The field has a tile drainage system installed at the depth of 1 m and spacing of 10 m. Three nitrogen rates of 90, 180 and 270 kg/ha was applied in the field study. Crop water uptake, evapotranspiration, and photosynthesis were also measured. This presentation will discuss the instrumentation and experimental methodology.

Estimation of Design Storms in Consideration of Climate Variability and Change

Nicolas Desramaut[1] and Van-Thanh-Van Nguyen[2]
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A "design storm" is a rainfall temporal pattern that is commonly used in the design of urban drainage systems. The 'synthetic' design storm of a specified exceedance probability is obtained from the intensity-duration-frequency (IDF) relationships based on the specified probability and duration. These models are computed based on rainfall records; unfortunately, they are therefore only accurate for the time frame of these data.

Climate variability and change will have important impacts on the hydrologic cycle at different temporal and spatial scales: from 5 min (for urban water cycle) to years (for annual water balance computation) and from few square kilometres (for urban watersheds) to several thousand square kilometres (for large river basins). In order to conceive drainage systems with lasting lifetimes, design storms should take into account these variations. However, if General Circulation Models (GCMs) are able to predict reasonably well future climatic parameters, their resolutions (generally ≥200 km and ≥1 day) are too coarse for their outputs to be used directly in impact studies of urban areas.

In view of the above-mentioned issue, this study proposes a statistical downscaling approach. First, a regression-based spatial downscaling (SD) method links the GCM large-scale climate variables with future local daily extreme precipitations. Then, based on scale-invariance properties of rainfall distributions, these annual maximum are temporally downscaled, to estimate sub-daily (as short as 5-min duration) extreme rainfalls. Hence, design storms can be generated from GCMs scenarios, and so, assessments of future trends for runoff peak flows and volumes for urban areas, performed.