ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING INDUSTRIAL CHEMISTRY AND

ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING



DOCTORAL PROGRAM IN ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING

Chair: Prof. Riccardo Barzaghi

The Doctorate in Environmental and Infrastructure Engineering has been operating since the academic year 2008/2009. The program introduces doctoral students to the world of research on key theoretical and technological elements associated with water, environment, hydraulic and transportation infrastructures, geology, as well as geomatics. In this context, the program is grounded on environmental, civil, and industrial applications where water is the primary unifying element. The doctorate program is characterized by a strong inter- and multi- disciplinary structure and is organized according to the following key thematic areas.

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- 2) Hydrology, hydraulic structures, water resources and coastal engineering, where the main research topics include: hydrology and water resources, with emphasis on the main physical processes of the hydrological cycle, water and energy budgets; hydrogeological hazard and mitigation strategies, including hydrological extremes, floods, droughts and precipitation, early warning operative systems, snow avalanching and flood risk; hydraulic networks engineering; and coastal engineering.
- 3) Environmental technologies, with focus on: water and wastewater treatment technologies (including disposal/reuse of wastewater, sludge management and disposal, anaerobic digestion processes; management and planning of environmental resources (including water quality modelling, knowledge-based decision support systems); solid wastes management (including Life Cycle Assessment of energy and resource recovery initiatives); phenomenology of the atmospheric environment and treatment of gaseous emissions; contaminated soils and their remediation.
- 4) Transport infrastructures and geology, with focus on: transport networks, including functional interactions with regional, national and international territory; sustainable development, in terms of dynamics of development and its relations with the infrastructure system; technological innovation, including methods and indicators for performance characterization of infrastructure construction and maintenance techniques;

hydrogeological risk, landslide hazard; water resources identification and management, pollution problems.

5) *Geomatics*, with focus on: physical geodesy and satellite geodesy; positioning and navigation; surface surveying with optical or other sensors, such as SAR, LIDAR; digital photogrammetry and image analysis; remote sensing; geographic information systems; cultural heritage reconstruction and archiving.

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REUSING EXISTING LAND COVER MAPS TO REINFORCE REFERENCE DATA FOR FUTURE LAND COVER MAPS PRODUCTION

Gorica Bratic - Supervisor: Prof. Maria Antonia Brovelli

Land cover (LC) is a physical material on the Earth's surface that affects many processes in nature. For example, it is considered one of the essential climate variables, but it also affects hydrological, ecological, and other processes. LC is modeled in the form of categorical maps, which are predominantly derived by machine learning from remotely sensed images. The development of LC maps is at an unprecedented level, given that there are high-resolution land cover (HRLC) maps at a global level.

A review of 16 existing global HRLC datasets showed that their accuracy varies between 60% and 80%. Only two recently released maps reported accuracy up to 86%. That is to say, there are still challenges to address to produce accurate LC in an efficient manner. One of the factors that directly affects the accuracy of LC is the quality of reference data. Reference data in LC production are used either to train machine learning algorithms or to validate classification outputs. In the case of the latter, probabilistic sampling is used to ensure robust accuracy assessment. Regardless of the reference data type, there are three main approaches to collecting reference data: in situ, photo-interpretation, and

using existing LC data. In situ is the most reliable approach, but it is extremely costly and therefore rarely used. The photo-interpretation approach has a good balance between cost and quality, and thus it is most commonly used. The use of existing LC data is the least expensive but also the least reliable approach.

The objective of this research was to develop an approach for providing reference data that maximizes reference data quality and minimizes costs. The research focused on providing reference data for global HRLC because they are the most common and most challenging LC data in recent years. The research behind this thesis examined the use of existing HRLC maps for reference data as a low-cost source of LC data and explored methods for improving their reliability. The initial focus was on validation reference data. After several exploratory studies related to the direct intercomparison of two HRLCs, spatial association of confusion between them, and manifold intercomparison, the idea of creating a Map of Land Cover Agreement (MOLCA) came up. MOLCA is an output of an intersection process of existing HRLC maps (Fig 1). The intersection process

combines the HRLCs by keeping only the areas in which all of the HRLCs agree and setting the pixels to null where at least one of the intersected HRLCs shows a different value. Most likely, manifold agreement of existing HRLCs happens in easy-toclassify areas. Therefore, one characteristic of MOLCA is that it is prone to easyto-classify areas. From a theoretical perspective, MOLCA tends to be highly accurate because there is a high degree of agreement among multiple sources of LC information. This was confirmed



Fig. 1 - Illustration of derivation procedure of the Map Of Land Cover Agreement (MOLCA) by robust validation of MOLCA using 1,050 photo-interpreted samples in one region in Africa. The validation showed an OA (Overall accuracy) of 96%, which is very high. Four out of seven classes had UA (User's accuracy) and PA (Producer's accuracy) above 90% too. The UA and PA of Grassland were close to 90%. Only the UA of Cropland was lower than the accuracy records of other classes, indicating an overestimation of the Cropland class. The Wetland class did not have any samples, so its accuracy could not be determined. The Bareland class only had one sample, so the accuracy figures for this class may not have been reliable.

High accuracy of MOLCA favored its use in the CCI (Climate Change Initiative) HRLC project of European Space Agency (ESA) for benchmark accuracy assessment in the first place, but also as a pool of training dataset with certain modifications. The CCI HRLC was focused on 3 macro-regions of the world subject to substantial climate changes - Amazon, Sub-Saharan Africa and Siberia. MOLCA derived for this project was based on six global HLRCs and one regional HRLC for each macro-region. It provided around 1.3 million training samples and around 94 billion samples for benchmark accuracy assessment. The samples referred to Bareland, Built-up, Cropland, Forest, Grassland, Shrubland, Water, and Wetland classes. In the role of training data, MOLCA was modified to broaden its legend with four forest types instead of a single Forest class. An auxiliary

MRLC containing these classes was used. MOLCA was then used together with samples collected by photo-interpretation in the classification procedure of CCI HRLC. In the role of reference dataset for accuracy benchmarking, MOLCA could not provide quantitative accuracy information because it is biased towards easy-to-classify areas. Nevertheless, it could indicate which classes of the dataset under the estimation had a high agreement with MOLCA and which did not. The low agreement of the dataset under estimation with MOLCA was considered useful, as it indicated significant misclassification. Due to the high number of samples in MOLCA, accuracy could be estimated in subregions of the region of interest, and spatial variation among regions of interest could be analyzed. Analyses of spatial variation are useful for identifying areas affected by lower accuracy. In addition to CCI HRLC, MOLCA was the exclusive source of training dataset in another use case, where a HRLC product with 78% accuracy was generated. This accuracy is comparable to the average accuracy of existing HRLCs produced based on more reliable training samples, such as photo-interpreted samples. In

another study, MOLCA was used

to refine training data collected

interpretation. The refinement

which samples were available,

and as a result, samples of two

classes were not available due

to their small size in the region

of interest. These classes were

significantly reduced the area in

in crowdsourcing by photo-

taken from the original training dataset and refined based on photo-interpretation. After the reference data was refined, the accuracy increased from 63% to 93%.

In summary, the main output of this research is the methodology to combine existing HRLCs to produce a new HRLC dataset with high accuracy, qualifying it as a trustworthy, stable, and low-cost reference dataset. The MOLCA methodology showed significant potential for supporting land cover mapping on a global scale, estimating that it could provide around a trillion LC samples globally. In particular, it can prove beneficial to state-of-the-art machine learning techniques such as deep learning, which require a massive amount of data. Nevertheless, it can be applied to any other algorithm and on a smaller scale too. There are some limitations and challenges to address, but the tests conducted so far indicate that further developing and refining this approach is feasible and worthwhile.

CIRCULARITY IN THE CONSTRUCTION AND DEMOLITION WASTE MANAGEMENT CHAIN

Federica Carla Carollo - Supervisors: Prof. Lucia Rigamonti, Prof. Francesca Ceruti

The PhD project results from a collaboration agreement between Lombardy Region, the ENEA - National Agency for New Technologies, Energy and Sustainable Economic Development research centre and Politecnico di Milano. The result of the three-year PhD provides a comprehensive study of the construction and demolition waste management (C&D) chain with the goal of fostering the circular economy (CE) in the construction sector through the implementation of tools useful to public administrations to encourage circular practices. A CE is essential in resource-intensive activities such as construction to reduce global impacts and preserve natural resources. The goal is achieved by implementing the Full-Environmental Life Cycle Costing (feLCC) methodology, which combines the Life Cycle Assessment (LCA) methodology with that of environmental Life Cycle costing (eLCC) through the monetisation of environmental impacts. Based on the study results, it is possible to suggest incentive mechanisms in favour of small and medium enterprises (SMEs) for the execution of private demolition works. C&D waste represents 45.5% of the total

production of special waste in Italy. Although the high recovery rate (78,1%), various regulatory, economic, technical, and cultural barriers prevent the widespread use of recycled aggregates (RAs) produced by C&D waste recycling activities. Among the limitations, market acceptance of products made using secondary resources as input material will only be ensured when their production costs are lower than those of virgin materials. Nevertheless, even more critically, the presence of impurities in the RAs and the difficulty in guaranteeing their consistent production preclude their use in structural concrete. To produce high-quality RAs, the waste entering the recycling plant must be as homogeneous as possible. Through selective demolition, a practice not very common in Italy, the materials can be carefully sorted, which is why it should be encouraged. The project was developed in four successive macro phases, the application of the eLCC, the application of the LCA, the monetization of the environmental impacts and finally the definition of the proposals for the incentive mechanisms. The first research phase aimed to apply an eLCC to Lombardy's C&D waste

management chain (Northern Italy). The functional unit chosen for the system is the demolition of a building per cubic meter (m3). The investigated system includes all management phases of inert waste originating from demolition activities, from its generation at the end of building life, during an ordinary or selective demolition, to the treatment phase in a recycling plant, till the market re-placing as RAs. The inventory is implemented for each process in the management chain, with two surveys issued to demolition companies and C&D recycling facilities, respectively. It is feasible to obtain complete data for seven case studies on the demolition phase (with a response rate of 10.61%) and two mineral waste recycling facilities (with a response rate of 7.41%). The LCA study of the selective demolition phase is performed under the same boundaries as the eLCC system. The system functional unit is the demolition of a cubic meter (m3) of the structure. The Life Cycle Inventory is developed using data from the eLCC surveys, which included the consumption of diesel, water, and energy, the typology and quantities of waste leaving the demolition site for recycling/landfill and on-site

reuse, and the distances that are driven. The model is developed using SimaPro 9.3 with the Environmental Footprint 3.0 characterisation method, which evaluates 16 impact categories. The union between the eLCC and the LCA occurs through the monetisation process of the environmental impacts. Four different monetisation methods are selected, i.e., De Nocker e DeBacker, Smith et al., Stepwise, and Environmental footprint. The monetised impact is calculated by multiplying the environmental impact indicator by the monetisation factor reported in the reference method. The final value of the eLCC is then added to the monetised impact to obtain the feLCC value. Starting from the results obtained, the incentive mechanisms for the benefit of selective demolition and the use of recycled aggregates are defined. In particular, the identified cost items on which it is possible to apply a discount on the cost incurred by demolition companies and recycling plants are the demolition project, the on-site reuse cost, the recycling fee, and the sale of RAs. The incentives are supposed to be payable by Public Administrations through tax relief and/or non-repayable grants. The recipients of these incentives are the SMEs for the execution of private works. The final step is to conduct a feasibility analysis on applying the incentives described above to real case studies. Multiple conversations with Lombardy Area workers have determined

which available funds might be spent for this purpose, and how much volume demolished every year can be entitled to incentives. In conclusion, although many challenges are experienced in gathering data appropriate for the eLCC, owing to organisations' lack of confidence in revealing sensitive data such as expenditures spent, the feLCC has proved to be a useful tool for identifying the criticalities of a value chain such as that of C&D waste. Using the available data, it is feasible to evaluate all the costs of the demolition chain (both internal and external through the monetisation of the impacts) and, as a result, develop some proposals to stimulate the market for recycled aggregates. The findings show that the average cost for demolition and C&D waste management is 7.04 €/m3. It was demonstrated that landfill expenses much outweigh recycling fees, and the cost of on-site reusing is equivalent to a landfill fee. However, it has the advantage of zero transportation expenses. The sensitivity analysis revealed that the total cost is lowered when the earnings from the sale of metal waste cover the expenses of transporting the other flows to the recycling plant or landfill. With the support of the LCA study, it has been revealed that when a more extensive breakdown of waste streams is accomplished, the outcome is opposite to the desired goal, i.e., increased environmental and economic impacts.

Recommendations are made for

operators in the sector on how to manage selective demolition better and which are the separable waste streams that bring greater benefits in both economic and environmental terms. A set of incentives is defined that can be directly used by public administrations in favour of SMEs in the execution of private works. The limits of the research provided are connected to the difficulties in gathering sufficient and representative data, and the geographical restriction to the Lombardy Area. As a result, one of the research's future directions is to expand the study to other Italian regions to gain an exhaustive case study of the current scenario and ensure that incentive programs are aligned throughout Italy and among all public administrations.

IMPACTS OF CLIMATE CHANGE ON HYDROLOGICALLY DRIVEN PASTURE DYNAMICS IN MOUNTAIN CATCHMENTS

Francesca Casale - Supervisor: Prof. Daniele Bocchiola

The aim of the PhD thesis work was the assessment of the potential effects of climate change upon the productivity of pasture in Italian Alps, focusing on Valtellina valley and the Gran Paradiso National Park (GPNP) in Valle d'Aosta region. The two study areas differ for extension, average altitude and climate: Valtellina covers an area of 2550 km² with an average altitude of 1930 m asl, while GPNP has an average altitude of 2340 m asl for 350 km² of extension. Cumulated annual precipitation goes from 800 mm/y in GPNP to 1400 mm/y in Valtellina, influencing the water availability in the two study areas. Climate change strongly affects the hydrological balance in alpine areas: the large increase of +2°C of temperature in the Alps, the double with respect to the global average, is causing a reduction of glaciered area (-30% since 1960), a reduction in snowfall against a larger rain share, and an anticipation of snowmelt season. These variations influence soil moisture, the available area and seasonality of pasture, and have consequences on biomass productivity.

To quantify the effects, some agro-climatic indices, related to climate and water availability, were introduced to summarize the effects, like i) evapotranspiration efficiency, the ration between actual and potential evapotranspiration (*ETeff/ETmax*), ii) relative evapotranspiration, the ratio between actual evapotranspiration and precipitation (*ETeff/P*), and water footprint (*ETeff/Y*), the ratio between actual evapotranspiration and pasture productivity.

A pasture model Poli-Pasture was developed here as module of the existing hydrological model Poli-*Hydro*, and it was used for the simulation of plants growth. Model simulates on a grid with different spatial resolution, of 1 km and 100 m respectively in Valtellina and GPNP, with a daily time step. Poli-Hydro simulates the soil water content, used as input for Poli-Pasture, that re-calculates actual evapotranspiration, vegetation coverage fraction and the corrected soil water content, used again by *Poli-Hydro* for the simulation of the next time step. Two different configurations in pasture modelling were used for the two case studies. For the first case study in Valtellina a single index species was considered, dividing the area in two altitude belts, under and above 2000 m asl, while for the second case study in GPNP two species in competition were considered in

each altitude belt. So, for the case study of GPNP, Poli-Pasture was corrected with a module, based on CoSMo model, for the simulation of inter-specific competition. The competition depends on bovines pasture liking, average temperature varying with altitude, solar radiation influenced by slope and exposure, and water availability. This module calculates a suitability index for each species considering these factors, then it simulates the relative presence of each species for each time step and in each cell of the study area. The community parameters that address the Poli-Pasture simulation are a weighted average of the species parameters, considering their relative presence. Starting from the information of collected samples in the study areas in fulfilment of the IPCC MOUPA project (*Interdisciplinary* Project for assessing current and expected Climate Change impacts on MOUntain PAstures, a

project founded by Fondazione

Cariplo for the study of climate

change effects on pasture in

the alpine area), some species

were chosen, among the most

abundant in Italian pastures, as

reference for the simulation of

pasture productivity. In particular,

Trisetum flavescens and Nardus

stricta were considered as index species in Valtellina valley, in the low altitude belt and in the high altitude one respectively, while *Trifolium alpinum*, *Dactylis* glomerata, Nardus stricta and *Festuca rubra* were considered representative of the pasture community in GPNP, in the same two altitude belts. The model was calibrated for the hydrological part through data of discharge in some river sections,

The model was calibrated for the hydrological part through data of discharge in some river sections, satellite data of snow cover area and data of snow depth. Poli-Pasture was calibrated for the Valtellina valley using ISTAT data of pasture productivity in the Sondrio province, and for the GPNP using satellite images of leaf area index (LAI). Moreover, model was validated with on-site collected samples of biomass. After the calibration of the model and the simulation for the present period, the model was used, for both cases, to project pasture productivity until the end of the XXI century, using the scenarios of the Fifth and Sixth Assessment Reports of IPCC, and considering a large number of global circulation models, specifically three for AR5 and six for AR6. Three representative concentration pathways RCPs for AR5 and four shared socioeconomic pathways SSPs for AR6 were used, for a grand total of 21 scenarios used in Valtellina, and 24 scenarios for GPNP. In response to the increase of temperature, the model projected a potential increase of pasture productivity, with some exceptions in low altitudes, in particular in Valtellina valley (until -31% for AR5 under 1100 m asl in

the period 2041-2050). In Valtellina vallev under AR5 the increase of total productivity is projected between +38% and +173% respectively for RCP 2.6 at the middle of the century (2041-2050) and RCP 8.5 at the end of the century (2091-2100), while under AR6 the increase ranges between +62% and +210% for SSPs 2.6 and 8.5 at the end of the century. In the area of GPNP under AR6 the increase of annual productivity ranges between +81% and +116% for SSP 7.0 at the middle of the century and SSP 8.5 at the end of the century. Here in low altitude belt the variation is contained, while in high altitude belt it is considerable. A large percentage increase does not correspond to a large increase in absolute value, considering an average fresh biomass productivity of 6.5 t/ha (12.9 t/ha in low altitude belt and 1.9 t/ha in high altitude belt) in Valtellina valley and of 3.6 t/ha (6.5 t/ha in low altitude belt and 3.5 t/ha in high altitude belt) in Gran Paradiso area during the present period. The large expected evapotranspiration demand in future, related to the increase of temperature, was satisfied in practice in Valtellina, notwithstanding the decrease of precipitation, thanks to a better use of water availability, more regular precipitation and increase of snowmelt at the beginning of the growing season. Differently, in GPNP area the lack of water availability from precipitation and

in GPNP area the lack of water availability from precipitation and snowmelt could be a limitation to growth. This is derived by the values of the agro-climatic indices: in Valtellina the increase of ET efficiency, the value of relative ET larger than 1 and the decrease of water footprint are opposite to the results in GPNP with the decrease of ET efficiency and water footprint, and the increase of relative ET. Generally, these indices have lower values in GPNP than in Valtellina. The result of the inter-specific competition simulation shows a larger presence of *Trifolium* alpinum(55%-59%) in low altitude belt and of Nardus stricta (71%-74%) in high altitude belt. In the future this condition will be exacerbated thanks to the better resistance of these species to high temperatures and drought conditions. Each species has a different nutritional value, so the general increase of biomass productivity is not related to an improvement of the value for pasture of bovines. The results provide preliminary evidence of altitudinal shift of pasturelands and of potential livestock, and thereby economic development, in the valley at higher altitudes than now. To conclude, differently from existing grassland models, Poli-Pasture allows analysing a wide area in high altitude catchment, thanks to the coupling with Poli-Hydro, specifically developed to consider complexity of climate and topography of alpine areas. The spatialization helps to analyse differences in future projections and potential effect in different territory of the study areas.

BIOTRANSFORMATION OF EMERGING CONTAMINANTS IN GROUNDWATER BODIES UNDER UNCERTAINTY

Laura Ceresa - Supervisors: Prof. Alberto Guadagnini, Prof. Monica Riva

In this thesis, we develop new modeling approaches to characterize the fate of emerging contaminants (ECs) and pharmaceuticals in groundwater bodies under uncertainty. To do so, we need to cope with the difficulties posed by accounting for the joint effects of multiple sources of uncertainty on the features of reactive solute transport in groundwater. These uncertainties span from the characterization of the spatial variability of specific hydrogeological properties of porous media, to the identification of potential reaction pathways (and ensuing mathematical formulations to predict the extents of reactions taking place in the aquifer), to the selection of appropriate parameter values embedded in such laws (e.g., in kinetic rate equations). The complexity of modeling frameworks is then exacerbated by the (usually) limited availability of empirical data, especially when dealing with ECs. In light of the difficulties posed by incorporating the effects of all the above-mentioned sources of uncertainty within a unique modeling framework prior to characterizing the system (bio) geochemical behavior, in this thesis we choose to focus on scenarios characterized

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by progressively increasing levels of chemical complexity. We start by considering a relatively simple geochemical system characterized by the occurrence of a conservative solute which migrates across a three-dimensional randomly heterogeneous porous medium. Underlying hydraulic conductivity fields are modeled according to the generalized sub-Gaussian (GSG) model, a novel conceptual framework which is increasingly recognized as capable of capturing documented non-Gaussian traits that cannot be explained through classical Gaussian models. Here, we address the effects of the parametric uncertainty related to the characterization of the spatial variability of underlying hydro-geological properties of porous media on key features of subsurface solute transport, including hydrodynamic (macro) dispersion. Corresponding closed-form analytical solutions are derived within the proposed modeling framework by resting on a first-order approximation (in terms of log-conductivity variance). Comparison of the analytical solutions against numerical estimates yields good agreement for degrees of domain heterogeneity that are

representative of the levels of

spatial variability contained within a single geological unit. The developed analytical solutions also reveal that solute dispersion across GSG fields is directly related to the heterogeneity structure of the host medium, and is markedly affected by the degree of departure from Gaussianity in the pre-asymptotic (i.e., non-Fickian) but not in the late time (i.e., Fickian) transport regime. As in our modeling framework deviations of log-conductivity fields from Gaussianity are modeled through the action of a unique parameter that ultimately governs the shape of our analytical solutions, the latter ones allow assessing key features of solute transport in a simple but effective manner. This allows saving computational time while ensuring satisfactory levels of estimation accuracy for all the considered scenarios.



Fig. 1 - Schematic illustration of the proposed diclofenac reactive network.

Relying on the proposed modeling framework is thus appealing to study problems of advectivedispersive transport in porous media. For instance, our analytical solutions can be used to perform preliminary analyses on solute plume evolution across domains that are representative of single geological units, where analytical macrodispersion coefficients may be employed to assess the extent of spatial spread experienced by solute particles around the mean plume (or particle) position. After introspecting the effects of porous media heterogeneity (and related uncertainty) on the dynamics of dispersive mass transfer, this thesis moves to consider a different scenario of increased geochemical complexity. Here, we address the effects of model and parametric uncertainties (as related to the conceptualization of complex geochemical reactions) on key outputs of a selected system, namely modelbased predictions of (reactive) solute concentrations. The corresponding workflow entails the derivation of an innovative modeling framework to interpret the occurrence of a complex reactive network involving the bio-mediated transformation of a selected emerging contaminant of high priority to the water

cycle (i.e., the pharmaceutical diclofenac; see Figure 1). The latter is (experimentally) seen to undergo a reversible biotransformation pathway in an artificially mimicked batch groundwater system under given (reducing) redox conditions. The proposed model is then calibrated in a stochastic context against a limited number of data. By doing so, we quantify the uncertainty associated with model parameters and predicted diclofenac concentrations. We also discuss the probabilistic nature of uncertain model parameters and the challenges posed by their calibration with the available data. In particular, our results reveal that our limited data availability might prevent an exhaustive characterization of all biochemical parameters involved in the proposed model. Since analogous challenges are commonly tackled when calibrating high-complexity models under uncertainty and data paucity for a variety of problems across different scientific/technical fields of application, enhancing stateof-the-art model calibration techniques in such contexts appears to be appealing for several disciplines beyond hydrology. With this spirit, in this thesis we lastly move to present a comprehensive model diagnosis and calibration approach which is developed in the context of a multiple model framework. The proposed strategy is based on pairing and applying a suite of quantitative tools starting from a prior diagnosis of multiple uncertainty sources and leading to parameter estimation and model selection in the presence of a limited number of observations. The methodology is illustrated through application to the above-presented reactive scenario involving diclofenac biotransformation in groundwater. Model discrimination criteria suggest that a simplified counterpart of the reference model is favored to interpret the available data, as evidenced upon the establishment of a balanced trade-off between the level of complexity of model conceptualization and associated estimation uncertainties. The proposed approach can also assist interpretation and prototyping of a wide variety of bio-mediated degradation models for recalcitrant compounds in soils and aquifers, as well as drive the design of future experimental sampling campaigns.

OCCURRENCE & FATE OF EMERGING CONTAMINANTS IN WASTEWATER, GROUNDWATER, AND DRINKING WATER

Salma Ebrahimzadeh - Supervisor: Prof. Arianna Azzellino

The presence of organic micropollutants (OMPs) in the aquatic environment is believed to pose risk to human health and ecosystems. Humans with different demographic characteristics and anthropogenic activities are the main OMPs producers in the aquatic environment. These substances are entered into the sewage networks and raw wastewater in wide ranges. In many cases, WWTPs are not capable of effectively removing OMPs and therefore these OMPs residuals are discharged into the surface water with treated effluent. On the other hand, these compounds contaminate the groundwater by leakage from the sewage networks and septic tanks, and exchange between groundwater and surface water. A serious problem occurs when contaminated surface water and groundwater are used as a source of drinking water. Due to the fact that the conventional drinking water treatments like coagulation, flocculation, and disinfection, are not specifically designed to remove these organic micropollutants, the OMPs residues remain in the treated water and thus the development and implementation of additional (advanced) treatment steps, like activated carbon,

ozonation, ultraviolet light, and membrane treatment, are strongly recommended although more expensive in operation and maintenance costs. On the other hand, reducing the amount of OMPs discharged in water resources could be more costeffective to tackle the risk of emerging organic contaminants than the additional advanced treatments. These reasonings are also in line with the current policy strategies to manage OMPs residues which are turned from reactive to proactive to more efficiently tackle the issue of the OMPs environmental risk. To support this from reactive to proactive transitions some relevant improvements should be pursued in the available knowledge on the occurrence,

fate, toxicity, human health and ecological risks of OMPs residues, in order to support the implementation of sourceoriented and use-oriented policy approaches, aimed to prevent and reduce pollution and to implement end-of-pipe measures to safely dispose and remove OMPs residues in a costefficiency perspective.

In this study, three different components of the OMPs environmental risk framework were investigated. The first component concerns the presence of OMPs residues in the effluents of wastewater treatment plants (WWTPs) that are significant polluting sources for surface waters. The second component is about



in the groundwater which is also very frequently used as a drinking water supply source, and the last component is related to the OMPs residues in the effluent of drinking water treatment plants (DWTPs) and the robustness of different water treatments against OMPs in DWTPs. Since exchanges between the aquifers, rivers and sewage networks can cause the contamination of surface water and groundwater, our results revealed that implementation in a WWTP of additional processes to remove OMPs will help to reduce their presence in surface water and groundwater resulting in less concentration of these compounds in the influent of drinking water treatment plants. This assessment might provide new insight into the implementation of end-ofpipe" (EOP) policies. Moreover, any improvement of the understanding regarding the OMPs load in the water cycle might be essential for the environmental risk assessment. Decreasing the amount of OMPs in water resources can be more cost-effective to tackle the environmental risk of emerging organic contaminants than the additional advanced treatments in DWTPs.

the presence of OMPs residues

In order to show the pattern of this research that was presented in the introduction section the graphical abstract was developed and added as follows.

CLIMATE CHANGE IMPACTS ON SURFACE HYDROLOGY AND AQUIFERS IN THE PO VALLEY. A FOCUS ON THE TICINO-ADDA CATCHMENTS

Flavia Fuso - Supervisor: Prof. Daniele Bocchiola

Climate change effects on the hydrological cycle of the Po Basin are already significant. Groundwater takes longer to respond to climate change with respect to surface waters, thanks to the soil and rock coverage. Nevertheless, also the groundwater is suffering, and the population growth and the increase in water demand is likely to cause the groundwater depletion in the following years. The management of groundwater resources requires the assessment of water exchanges between surface and subsurface bodies, making thus necessary the development of a holistic approach to safeguard water resource availability in the future. This work aims to frame a comprehensive modelling chain made up of climate, hydrological, hydraulic, and hydrogeological tools, to improve the present state of the art of hydrological modelling within a climate change context.

The physically based hydrological model *Poli-Hydro* was set up for the study area nested in the Po Basin, supported by weather, snow, and hydrological data validation. It was fed with Global Circulation Models'(GCMs) outputs in response to several emission scenarios provided in the latest Assessment Report

6 of the Intergovernmental Panel on Climate Change (IPCC) to simulate the future hydrological conditions. Then, it was coupled with an HECRAS hydraulic modelling to provide the hydraulic characterization of the main rivers of the study area. To gain reliable results and to increase confidence in climate and hydrological projections, an *ex post* validation of GCMs was also pursued. The methodology was then applied to a CAP Holding project aiming at assessing the hydrological flows in Lombardy Alpine rivers and their connections with the underground aquifer under potential climate change scenarios, to delineate sustainable groundwater management strategies.

WATER SCARCITY: MODELING CONFLICTS AND SYNERGIES IN WATER USE

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Water is at the core of many global and regional challenges. Interactions between human systems and water systems contribute to shaping sustainable development. Hydrosocial interactions are often expected to ignite when water security is impacted. In this sense, measuring water availability in relation to its multisectoral utilization can be a way to guantify the effect of humanwater interactions on sustainable development. This thesis investigates water scarcity as a quantitative representation of human-water interactions, and the possibility of reversing this paradigm, so to transform water scarcity indicators in design tools for more hydrologically conscious sustainable development strategies.

The core research in this thesis is based on modeling the daily water balance of the active soil layer, where "vertical" exchanges between soil moisture and vegetation take place. Green (precipitation-generated) and blue (irrigation) water fluxes are computed, and thus green and blue water scarcity indicators are derived. The advantage of this is that variations in these indicators can be computed by modifying both inputs to the indicators and to the model, increasing the range of assessable scenarios. A series of applications of this framework is presented, progressively moving from explorations of competitive/conflictual humanwater interactions to the design of synergistic human-water interactions.

Conflictual water use is addressed as different production sectors or social strata competing over water and analysed for the Democratic Republic of Congo (DRC), where alluvial mining represents an important income alternative for subsistence farmers, but with several socio-environmental impacts. Water scarcity is used to quantify impacts of mining on natural resources and assess the potential relevance of these resources to the food system, given the chronic food crisis of the country. Despite the richness in natural resources of the DRC, mining has effects on ecology, economy, and society. Resources and efforts currently put into the mining industry may alleviate the food crisis if diverted towards a more structured and resilient food system. The illicit trafficking of diamonds and their use to finance wars contribute to nullify the potential of mining as an income alternative for subsistence farmers.

Indeed, the role of environmental

stress in violent conflicts is highly debated, but also of high interest, especially where water and land have a primal role in the local population's livelihoods. Whether and how water scarcity relates to conflicts is investigated in the thesis for the Lake Chad Basin, in Central Africa, using different declinations of water scarcity in two statistical analyses, with a critical modeling interpretation to broaden the hydrosocial framework. Complex waterrelated interdependencies are unveiled, acting on different scales beyond the main political conflict drivers, and mediated by specific water utilization processes and conflict mechanisms. Many of these interdependencies are related to the importance of water for human sustenance. Therefore, the water-food nexus is further investigated in relation to urban conflicts in Central America. The results show how drought induces water scarcity in rural areas, producing food insecurity, which is then propagated through the internal trade network as a social stressor in major cities. To move from conflict to synergy, water scarcity indicators are progressively used as an impact measure of, a limit to, and a design parameter for potential sustainable development

strategies, for instance to understand impacts of largescale afforestation projects in the tropics. By simulating the introduction of these new forests, their hydrological impact can be assessed, and new water competitions, e.g. with the agricultural sector, quantified. The results show that new forests would only be partially sustained by rainfall, increasing water scarcity both locally and downstream. This aspect of proximal and remote impacts is crucial in the following case study, which combines a water productivity-based design of agricultural expansion with a water scarcity impact assessment. This analysis is performed with the target of meeting sustainable development policies in the transport sector, especially in civil aviation, where biofuels are projected to power up to half of world traffic. Areas are mapped where harvesting biofuel crops is environmentally and socially sustainable and where water is locally sufficient to support it. The areas are then allocated to different crops according to the efficiency in water use. Even with these measures, the results show that only part of the projected biofuel demand can be sustainably satisfied, and that significant local-to-global water use tradeoffs emerge. It is therefore necessary to use water scarcity directly as the design parameter for hydrologically sustainable development strategies. Thus, a framework is developed to identify and quantify

hydrologically sustainable changes directly accounting for downstream effects. The method consists in simulating hydrological alterations caused by agricultural expansion, and using these simulations to progressively filter out areas where the expansion generates water scarcity. This method is tested on expansions of coffee plantations in Kenya, a transformation encouraged by local policies, and it successfully selects areas where this expansion could happen at negligible costs for other water users. The physically robust, and thus transparent and understandable approach used by this framework makes it a potentially useful methodology for sustainable agricultural development planning. Similarly, the biophysical nature of water scarcity indicators is leveraged to assess the global potential of agrivoltaic, an emerging sustainable development strategy combining energy and food production. After quantifying the current status of land competition induced by utility scale photovoltaic plants, the hydrological mechanisms generated by the superposition of solar panels on cropped surfaces are investigated. A trade-off emerges between a slowdown in photosynthesis and a decrease in green water scarcity, producing a nonlinear response in terms of crop yield. Indeed, yield variations associated to agrivoltaic turn out to be positive or negative depending on the crop and the location. This, combined with information on social sustainability, land availability and

the presence of infrastructures, allows to use yield variations as a criterion to identify areas where agrivoltaic could provide advantages for both food and energy.

Results across the case studies show that similar approaches can be applied to a broad range of applications, moving from waterenergy-food nexus strategies to agricultural transitions and socio-hydrological issues. While there is room for improvement towards a further formalization of this framework, the flexibility that makes it applicable to such a variety of instances also makes it an exportable and upscalable analytical lens. On a more epistemological perspective, the research activity behind the series of interconnected research items presented here has been a wider process of formation through transdisciplinary collaboration, with a strong reflective component. The thesis highlights on one hand the importance of overcoming siloing barriers between scientific sectors, and the crucial role of collaboration between academia and local communities to guarantee, through co-design and co-creation, the validity and the applicability of sustainable development strategies based on state-of-the-art scientific tools and expertise.

EXPERIMENTAL AND NUMERICAL MODELING OF HYDRAULIC ROUGHNESS INDUCED BY FLOODPLAIN VEGETATION

identifying the models that best

represent the experimental

Lisdey Verónica Herrera Gómez - Supervisor: Prof. Marco Mancini

Vegetation plays a vital role in riverine ecosystems, providing food and habitat for a diverse range of animal species, as well as stabilizing soil and purifying water. However, from a river hydraulics perspective, the presence of vegetation growing along the banks and floodplains creates additional drag forces as the water passes, contributing to an increase in the flow resistance. As a result, it is important to accurately estimate the hydraulic roughness caused by vegetation to properly conduct flood analysis and river management activities aimed at risk mitigation and protection of river ecosystems.

This thesis examines the impact of floodplain vegetation, specifically the arboreal, on flow resistance through a combination of experimental and field studies, as well as numerical simulations. Considering the numerous vegetation roughness models that exist in literature, the first part of this work focused on experimentally validating these models in a flume using wooden cylinders to represent the vegetation. Two diameters and two spatial distributions were tested under submerged and emergent flow conditions. The resulting analysis allowed

measurements for the given flow conditions. During fluid-structure interaction, the forces acting on the flow can cause vibrations in vegetation, which depend on the vegetation's mechanical properties and dimensions. These vibrations can result in additional energy losses, potentially modifying the roughness coefficient. Using an experimental model, this study analyzed the vibration of vegetation, represented by cylinders, and its effects on energy losses employing the theory of structural dynamics. Most experimental approaches typically investigate either rigid or flexible vegetation separately. However, since floodplains are characterized by a mixture of species such as grasses, crops, bushes, and trees, a series of experiments were conducted to examine the flow resistance due to mixed vegetation. The experimental set-up included wooden cylinders (rigid) and synthetic grasses (flexible). Roughness coefficients were determined individually for rigid, flexible, and mixed vegetation to investigate the importance of mixed vegetation in flow resistance analysis.

To apply the laboratory findings to the river scale, this study evaluated roughness coefficients due to arboreal vegetation in the Piave river in Italy applying the vegetation roughness models that performed best in the laboratory study. As a result, a map with the spatial distribution of roughness coefficients was produced. Moreover, a continuous water depth measurement system installed in the field allowed determining the floodplain hydrographs for a flood event that occurred in December 2020. Finally, this thesis used a twodimensional hydrodynamic model to perform numerical simulations and validate vegetation roughness models at the river scale. The simulations focused on the arboreal vegetation and studied the flooding event that occurred in the Piave river in October 2018. The results of the vegetation roughness models were compared with those of the conventional approach, which uses a constant Manning coefficient to define roughness. Furthermore, this study showed the effect of vegetation density on water levels and the extent of flooding.

Overall, this research aims to improve the understanding

of the effects of floodplain vegetation on flow resistance analysis, using a combination of experimental, field and numerical studies at both laboratory and river scales.

SPATIAL COMPOUND EVENTS IN A NETWORK FRAMEWORK

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One of the most challenging expressions of atmospheric circulation is compound events. They are characterized by one or multiple dependent variables that merge and cause extreme impact. One way in which this can be declined is spatial dependence. The thesis aims to analyze the spatial dependence between binary time series of precipitation at a continental scale. So the dissertation is on two main topics. The first is to find a measure of dependence between binary variables that can account for the temporal autocorrelation implicit in binary precipitation series and that can characterize the combination of states in which dependency is present. The second is to analyse the structure of spatial dependence using complex network theory. We answered the first question by proposing two methods that consider the precise characterization of dependence, the temporal autocorrelation, and the significance of the results. The first method compares the joint probability with the product of the probabilities of the four possible state combinations and applies an independence test. The second method estimates a threshold of the interest factor.

This brings many advantages in studying the dependence of only one combination of states over the \$\phi\$ correlation coefficient. The threshold on the interest factor is used to design the extreme precipitation network in Europe and in the Mediterranean

Europe and in the Mediterranean area. Network analyses are carried out to understand the topological structure and its relation with the climate areas. Moreover, the European network is compared with a spatial null model to understand the nature of the spatial dependence (due to distance or due to synoptic circulation). The analysis suggests that the type of dependence created in the synoptic-scale territory is an overlap between dependence due to proximity and dependence due to more complex phenomena, which are unexpected. The dependence on distance is not relevant. These results give insight into how the tool of network science can be really useful in understanding complex phenomena such as compound events.

ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING

INTEGRATED WATER MANAGEMENT STRATEGIES IN RIVER BASINS: HYDRAULIC RISK AND ECOLOGICAL VALUE

Franco Raimondi - Supervisor: Prof. Gianfranco Becciu

Rivers have been one of the main resources for the development of civilizations since ancient times, first as a source of livelihood and for agricultural activities and later as a communication route and source of energy. However, the man-river relationship moved from being an equal and symbiotic one, based on the use of resources without degradating the environmental integrity, to one in which man has assumed the total control. Especially over the last century, the race for progress and the demographic boom has led to uncontrolled and unprecedented exploitation of water resources, resulting in quantitative and qualitative impoverishment. The urbanization growth and soil sealing, the construction of dams, mini-hydroelectric plants and bridges have altered the river environment at the hydrological, morphological, and ecological level, increasing the flood risk and worsening the chemical and ecological water quality. In addition to anthropic pressures, there are also those related to climate change. The traditional water management approach has focused above all on the mitigation of hydraulic risk without considering the quality aspects. However,

this approach, based on the stormwater conveyance from urban areas as quickly as possible and the channelization of the rivers, did not lead to a significant reduction of flood risk.

Since the 2000s, the European Community has adopted the Water Framework Directive and the Floods Directive, in which the river basin is identified as the suitable territorial unit of measurement for the implementation of strategies aimed at mitigating flood risk and improving water quality. New ways of water management include river restoration and Sustainable Urban Drainage Systems (SUDs). The first consists of restoring the typical structures and shapes of natural rivers, and the second of recovering the natural processes involved in the water cycle. These two types of strategies, however, are often used separately and for the unique purpose of hydraulic risk mitigation.

The aim of this research is instead to propose an integrated approach of the two strategies, highlighting their ability to mitigate the hydraulic risk at the basin scale and at the same time to improve chemical and ecological water quality and provide ecosystem services, working as multi-objective strategies. The integrated approach is applied to a real case study, the Seveso River Basin, north of Milan, chosen for its historically known criticalities concerning floods and poor environmental and water quality. Results show the effectiveness of the proposed river restoration interventions in hydraulic risk mitigation, with a significant reduction of potentially flooded areas, and improvement of the river ecosystem. However, it is necessary to act also upstream reducing stormwater peak flow rates and volumes discharged to obtain more efficient results. For this purpose, two different stormwater control strategies were investigated.

The flow-limited one is based on the imposition of a maximum admissible discharge rate, while the volume-limited one is based on the introduction of retention basins capable of infiltrating into the subsoil. The analysis shows that the volume-limited approach can provide more effective results.

SUDs are part of this approach and, among the various types of SUDs, permeable pavements, green roofs, bio-retention areas, rain gardens, and swales have been considered in the present research project. A comparison among the various types of SUDs, aimed at the reduction of discharged stormwater volume, in the case of two different types of natural soil permeability (high and low) shows that permeable pavements and bio-retention areas are the most efficient techniques.

SUDs strategies were then applied to the case study, evaluating the effectiveness of reducing peak flows and volumes first, at the municipal level, with permeable pavements, and then, at the neighborhood scale, comparing scenarios that contemplate the use of a single type of SUDs or a combination. In both cases, significant reductions were obtained, up to the complete retention in the case of integrated use of all SUDs types.

The analysis of the combined effect of river restoration and SUDs highlights the further decrease in potentially flooded areas that the SUDs interventions, applied to a very small area of the river basin, can determine.

Benefits in implementing SUDs and river restoration are not limited to hydraulic risk reduction. Indeed, the same scenarios considered for the neighbourhood scale analysis were compared in terms of removing pollutants and through a cost-benefit analysis. The results confirm that the simultaneous integration of multiple SUDs leads to total pollutants removal and can significantly reduce energy consumption and CO2 emissions in the long term, demonstrating the multi-objective behaviour of these strategies. The contribution of this research consists in the analysis of integrated strategies of river restoration and Sustainable Urban Drainage Systems. The effectiveness was tested by the application to a case study, showing that a significant reduction of the flood risk and a simultaneous improvement of the river ecological and chemical water quality, linked to multiple additional benefits, can be achieved.

CRYOSPHERE HYDROLOGY IN A CHANGING CLIMATE

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Consciousness of climate change and its detrimental effects on cryosphere is quite widespread between public opinion. As these effects become more evident from year to year, the theme of climate change and is more urgent so much that its mitigation and adaptation measurements are getting a priority in the agenda of worldwide governments. Indeed glaciers are one of the most suitable and visible example of climate change effect. In contrast to temperature, which have a strong seasonal and annual variability, and then its increase is more difficult to be touched by hand, glacier retire is (relatively) easy to measure and can be seen evidently also by non specialists. In Alps mass loss is in the order of -0.7 m.w.e. a⁻¹, and as their thickness is relatively small if compared to Himalayan glaciers, this leads to also relevant area change, i.e. -50% from 1850 to 2000, and to the fragmentation of larger glaciers in smaller ones. Even if highly dependent on seasonal precipitation regime, and then exposed to relevant annual variability, also the reduction in snow cover can be considered as a popular symbol of climate change: lack of snow indeed directly affects local economy in mountain areas and has already brought

to the cancellation of main wellliked skiing competitions and to the definite closure of many skying area whose presence is now testified only by the ruins of lift facilities. With respect to depletion of ice and snow cover, permafrost degradation in Alpine area is less discussed by media but it's a relevant topic in high latitude regions where perennial permafrost degradation, even in unpopulated area, could have enormous consequences on global carbon cycle. As a matter of fact, if cryosphere degradation is well known, the quantification of the phenomena and its consequences are still to be deepened and partially unknown. Here we just enumerate some of the main critic aspects related to cryosphere degradation. We already mentioned the economic losses in mountain tourism given by snow ablation but, even if they might be the ones with highest media impact, they are not the most relevant in absolute term. The formation of snowpack during winter in alpine area delays discharge to spring-summer period when melting occurs, benefiting agriculture as crop water requirements are indeed higher during that period. Higher temperature leads to lower snowfall and earlier ablation, with

the consequent risk of drought

during crop's maximum water demand. Glaciers, when present, are nowadays buffering lack of water like it happened during 2003 and 2022 but as soon as their area will drastically reduce droughts might be even tougher. Furthermore glaciers' degradation is also relevant in terms of direct threat to people life. Only during summer 2022 several tragedies occurred within a few weeks in the Alps: the detachment of seracs from the Swiss side of Grand Combin which instantly killed 2 climbers, and the failure of the Marmolada glacier, which caused 11 casualties. Also, permafrost degradation can be very dangerous in mountain area: it can trigger devastating landslides as most reliably occurred in Val Pola in 1987 and in Val Bregaglia in 2017. Degradation of permafrost in subartic area, with some exceptions, does not cause violent and spectacular events, but as it entraps an estimated amount of CO2 equal to 2.5 times the amount of CO2 stored in atmosphere, its degradation itself could be a main driver of climate change in the future.

Previously we reported that cryospheric cycle degradation due to climate change is still quite a challenge to be assessed, and that this obstacle can be largely related to data availability. As the evidence of glacier retire is higher than the evidence in snow cover reduction, which is in turn higher than permafrost depletion, the availability of data describing these phenomena follows the same diminishing path. Glacier retire, at least in terms of area reduction, can be relatively easily assessed with satellite images. Snow cover can also be detected with remote sensing, but measurements of depth require the presence of a weather station, where the value can be measured from the ground with a rod or a sonar placed on the top. Still these measurements do not provide the amount of snow water content, which requires measurements of snow density, which are quite rare in literature. Furthermore, snow depth and density is much affected by variables like slope, wind, solar exposure and then punctual data are difficult to be spatialized consistently. Regarding permafrost, most sophisticated sensors have to be use in order to get indexes of the areal extension, while geophysical method of electrical resistivity tomography, geocryological and drilling boreholes must be applied to assess permafrost extension in vertical direction. Even in the case where abundant direct measurements are available, the spatial variability and the complexity of the physical phenomena are such that a consistent quantitative assessment of cryospheric cycle could be hard to get. Discharge measurements in a

downstream section, especially if combined with a hydrological model, are so an useful tool for scholars studying cryosphere as they provide precious data at a relatively cheap cost regarding amount and timing of cryosphere depletion.

Here we report three case study regarding cryosphere impact on hydrology and its evolution during climate change. The first and main focus is related to Valtellina Valley in Italian Alps, where within the project Idrostelvio (2010present) a set of 11 hydrometers were installed in natural streams at high altitude, glacierized basins. As measurements of discharge were done by operators through the years, it was possible to assess rating curve was assessed for each station. Then values of discharge were obtained used to calibrate the hydrological model Poli-Hydro implemented for 1995-2022. This provided us an assessment of snow/ice melt contribute to discharge and also an assessment of glacier volume variation, with a focus on Forni Glacier, the second largest of Italy. Second study is an analysis of snow cover in Ossola Valley of Piedmont region of Italy. Here 2 datasets were available: a long term (1930-2021) series from 9 stations of snow depth, temperature and precipitation, and a recent (2007-2021) dataset of snow depth and density for 47 stations. The former was used to assess (negative) variation of snow cover in the area due to increasing temperature, while the latter gave us data about trend of density and Snow Water Equivalent with respect to

season. In particular we found date of peak of SWE to be delayed with altitude for 6 days every 100 m vertical jump. Third study is related to a high latitude basin, the one of Suntar River in Siberia, where due to large seasonal temperature variation and flat land, glaciers are small, and ice formation is mostly seasonal and given by permafrost and aufeis, hydrological model *Poli-Hydro* is here modified including heat flux equation in order to take into account variation of active layer given by permafrost formation/ ablation. Heat parameters were calibrated vs discharge measured by a hydrometer at basin closure section, providing monthly NSE equal to 0.7.

In Idrostelvio project and Ossola Valley study, also thanks to the relative abundance of data available, it was possible to stress the effects of climate change: indeed we model/observe strong reduction of ice cover in Stelvio Park, while in Ossola relevant change of long term snow cover is assessed. In Suntar basin, due to the peculiarities of the region, where there is a much higher seasonal temperatures variation with respect to Alps, and also due to the poorness of data, making impossible to perform refined analysis, the effects of climate change were not detected.

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DEVELOPMENT OF A σ -ONLY TWO-FLUID MODEL FOR THE PREDICTION OF PSEUDO-HOMOGENEOUS SLURRY PIPE FLOW

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Introduction

Slurry pipelines are one of the most widely used methods to convey solid particles. They are used in a variety of industrial applications, ranging from mining engineering to pharmaceutical engineering. Much attention has been dedicated to slurry pipe transport in the last decades, in order to ensure the safety, efficiency and production of the process. Initially, the researchers used to run tests at the laboratory scale and, based on these data, developed empirical predictive correlations or mechanisticbased models. About 30 years ago, thanks to the development of the numerical algorithms and the computational power, **Computational Fluid Dynamics** (CFD) became an effective tool to locally investigate the physical mechanism governing the slurry pipe flow for both academic community and engineering practices. Nowadays, CFD is used as much as the traditional approaches. In this regard, this thesis mainly focuses on the improvement of the CFD approach through the in-depth assessment of the predictive capacity of the models. Particularly, reference is made to the β - σ two-fluid model developed by my supervisor and co-workers after ten-year-long research[1]

Mathematical model

The β - σ two-fluid model, as it was the IPSA of Spalding[2], is obtained through the first double-averaging scheme, in which all solved variables are the time-averaged of the volumeaveraged ones. In this thesis, it was assumed that the slurry pipe flow is statistically steady and isothermal, as that the carrier fluid is incompressible. Therefore, conservation equations of both phases and closure equations read as below.

$\nabla - \Phi_1 \rho_s U_q - \nabla \cdot \left(\frac{\gamma_s}{\sigma} \nabla \Phi_0\right) = 0$
$\nabla - \Phi_1 \rho_1 U_1 U_1 = - \Phi_1 \nabla P_1 + \nabla \cdot \Phi_1 [(\rho_1 + \rho_2) \nabla U_1]$
$+ \Phi_{1,\theta_{1}\Sigma} + M_{M}^{c} + \nabla \cdot \left(\frac{d}{c} U_{1} \nabla \Phi_{1}\right)$
$\boldsymbol{M}_{ii}^{d} = \frac{3}{i q_{i}} \boldsymbol{\Phi}_{ij} \boldsymbol{\eta} \boldsymbol{C}_{ij} [\boldsymbol{U}_{i} - \boldsymbol{U}_{i}] (\boldsymbol{U}_{i} - \boldsymbol{U}_{i})$
$C_{g} = \max \left[\frac{34}{4c_{m}} (1 + 0.15) R d_{m}^{0.637}, 0.44 \right]$
$Re_{\mu} = \frac{mi_{\mu}(D_{\mu}E_{\mu})}{E_{\mu}}$
$\mu_{\rm in} = \mu_0 \exp\left\{ \frac{z + s}{s} \left[\frac{1}{ z - \theta_0 } - 1 \right] \right\}$

Where: $\rho_{\nu} \phi_{\nu} U_{\nu} \mu_{\mu}$ and μ_{ν}^{t} are the density, the locally averaged volume fraction, the locally averaged velocity vector, the viscosity, and the eddy viscosity of two phases; the subscript kindicates either solid phase s or liquid phase I; P_i is the locally averaged pressure, shared by the phases; q is the gravitational acceleration vector; and M^{d}_{μ} is the generalized drag term. C_d is drag coefficient; R_m is the particle Reynolds number characterized by a peculiar friction parameter μ_m which is originally developed

by Cheng and Law[3]; d_p is the volume-equivalent particle diameter. It should be noted that $\mu^t_{,c}$ can be calculated through the two-phase k- ε standard turbulence model for high Reynolds number flows and

$\mu_s^t = \frac{\rho_s}{\rho_l} \mu_l^t$

(1)

65

(7)

145

03

10

Obviously, two main numerical coefficients which need to be calibrated, namely β and σ , characterize the effect of particle shape on the friction and turbulent diffusion of particle, respectively.

Results and Discussion

Firstly, the role played by two calibration coefficients of the model, β and σ , on different features of the numerical solution is clarified by an extensive sensitivity analysis. An effective calibration strategy for determining the appropriate values of β and σ is proposed and verified by considering three experimental test cases over a wide range of physical conditions. Very importantly, the suitability of β and σ outside the calibration conditions is investigated in terms of changes in pipe size, particle material and in-situ solid concentration. Based on the above analysis, it is found that, although the performance of the β - σ model is overall satisfactory, some physical features of the flow at high concentration cannot be correctly captured (Figure. 1). Therefore, efforts involved going beyond the β - σ framework. Bearing this in mind, the whole experimental data reported in the open literature concerning pseudo-homogeneous slurry pipe flows, are combined and



Fig. 1- Validation of the model with σ =0.50 and β =0.25 for glass bead slurry[4]: (a) exemplary comparison of concentration profiles for Vm \approx 3 m/s and different average concentrations; (b) parity plot of predicted vs measured hydraulic gradient.



Fig. 2 - Prediction of σ -only model against the the experimental data with σ =0.75 at C_{_{III}} < 30\% and Vm > 2V' $_{\sigma}$

made comparable to create a the slurries can be explained reference database. In-house in a coherent manner if the specific gravity of the mixture is measurements performed during a stay at the University of Coimbra, less than 1.5 (more or less 30% which basically confirmed earlier in-situ concentration by volume). data collected at the same lab, These considerations are the were also added to the database. basis for developing a new σ -only This allows assessing that the model, whose main advantage dissipation characteristics of compared to the β - σ one is the higher robustness owing to the presence of a single calibration coefficient. At the same time, the applicability limits of the σ -only model are more restricted, and

the high concentration cases in which the performance of the earlier β - σ formulation was poor were excluded. Having a single calibration parameter alleviates the calibration procedure, and also slightly improved the accuracy of the model in the restricted applicability range (Figure 2). Finally, the σ -only model, originally developed in the commercial code PHOENICS, was implemented in the open source code OpenFOAM so that it can be distributed freely to the scientific community.