





Chair:  
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## DOCTORAL PROGRAM IN ENVIRONMENTAL AND INFRASTRUCTURE ENGINEERING

The Doctoral Program in Environmental and Infrastructure Engineering has been operating since the academic year 2008/2009. The program is dedicated to exploring crucial theoretical and technological aspects related to water, the environment, hydraulic and transportation infrastructures, geology, and geomatics. In this context, the program is grounded on environmental, civil, and industrial applications where water is the primary unifying element. The doctoral program stands out with its remarkable inter- multi- and trans-disciplinary structure, fostering a comprehensive approach to research. It is carefully designed around the following three key thematic areas, collectively providing a comprehensive platform for advanced research and expertise in the field of Environmental and Infrastructure Engineering.

**Area 01. Water Science and Engineering.** This area delves into the realm of hydrology and water resources, with emphasis on the main physical processes of the hydrological cycle, water and energy budgets. It also includes the study of hydrological hazards and strategies for their mitigation, hydrological extremes, floods, droughts and precipitation, early warning operative systems, snow avalanching and flood risk; hydraulic networks engineering; and coastal engineering.

**Area 02. Transport infrastructures and Geosciences.** This area focuses on the dynamic interactions between transport networks and regional, national and international territories. Sustainable development, encompassing dynamics of development and their relations with infrastructure systems, is a key aspect. Technological innovation, including methods and indicators for performance characterization of infrastructure construction and maintenance techniques, is also explored. Furthermore, this area encompasses research on hydrogeological risk, landslide hazard; water resources identification and management, and pollution problems.

**Area 03. Environmental and Hydraulic Engineering and Geomatics.** Research in this area covers a wide range of topics. It encompasses water and wastewater treatment technologies, including disposal and reuse of wastewater, efficient sludge management and anaerobic

digestion processes. Management and planning of environmental resources, such as water quality modeling and knowledge-based decision support systems, are also explored. Solid waste management, including evaluating energy and resource recovery initiatives through Life Cycle Assessment, is another focus. Other subjects covered in this area are computational and experimental fluid dynamics, fluid-structure interactions; river hydraulics; sediment mechanics; hydraulic risk assessment and management; flow and transport processes in porous systems; hydraulic networks, hydro-energy; oil and gas development and applications, physical geodesy and satellite geodesy; positioning and navigation; surface surveying; digital photogrammetry and image analysis; remote sensing; geographic information systems and cultural heritage.

The doctoral program has been designed to address the intricate and diverse research questions surrounding the complex interplay between the water sphere and the key evolving anthropogenic activities responding to the needs of modern society. PhD students will be skilled in an interdisciplinary and multi-sectoral environment and will gain excellent communication, management and research skills. They will acquire a set of skills and a knowledge base transferable to a range of real-world challenges related to ecosystem services. These skills open up significant opportunities for PhD candidates in academia, as well as in private and public organizations. Career perspectives include opportunities at Universities, Research Centers, public bodies and Authorities, as well as private companies / industry. Small and medium size enterprises (SMEs) which cannot afford the

development of an in-house specific know-how program may also require such highly professional profiles to guarantee critical innovation and competitiveness.

### LABORATORIES

An integral component of the Doctoral Programme is the presence of our state-of-the-art Laboratories. These encompass various domains, including the laboratory of (i) Hydraulics "Gaudenzio Fantoli", (ii) Environmental Engineering, (iii) Geodetic and Photogrammetric measurements, (iv) Applied Geophysics measurements, (v) Transport Infrastructures. These laboratories, linked to the strategic issues characteristic of the different territorial areas, are an indispensable and valuable tool for the development and implementation of the research activities of our PhD candidates.

The Department's Laboratories are also headed by experimental platforms allocated for logistical needs at industries, plants, research centers, and experimental sites. Additionally, our doctoral program relies on computational infrastructures dedicated to software development and to interdepartmental laboratories, such as GEOLAB (Geomatics and Earth Observation Lab), SoLINano-LAB (Solid-Liquid Interface Nanomicroscopy and Spectroscopy Lab) and CFDHub@Polimi (Computational Fluid Dynamics Lab). These laboratories and computational resources not only enhance the research capabilities of our doctoral students, but also facilitate inter- and cross-disciplinary collaborations, enabling our students to make significant contributions in their respective fields and to address complex challenges in their research activities.

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## FLOOD DAMAGE ASSESSMENT TO POWER GRIDS

Panagiotis Asaridis – Supervisor: Prof. Daniela Molinari

Co-Supervisor: Prof. Francesco Di Maio

Flood damage assessment is a critical aspect in any decision-making process on flood risk management. For this reason, reliable tools for flood damage estimation are required for all the categories of exposed elements. Power grids are critical infrastructures (CIs) that constitute the lifeblood of societal and economic development. They can suffer significant economic losses in case of floods. Moreover, floods significantly affect their functionality in terms of frequency, magnitude, and duration of power outages triggered by the failure of certain components. These outages can lead to widespread impacts on households, businesses, industries, or agricultures, and on other infrastructures dependent on electricity for their functioning. Despite this, modelling flood damage to power grids (and more in general to CIs) is still a challenging task. In fact, the current procedures for flood risk assessment generally neglect, or estimate with over-simplified assumptions and tools, damage to them. This is due to (i) the structural and dynamic complexity of infrastructure networks, (ii) the lack of knowledge to investigate damage mechanisms, and (iii) the paucity

of data to calibrate and validate damage models. Given the lack of a consolidated methodology for comprehensive flood damage assessment to power grids, this dissertation takes up the challenge to address this topic. The objective is twofold: (i) to enrich the knowledge on damage mechanisms and (ii) to supply a modelling and simulation tool that focuses on the estimation of flood damage to components, the arising cascading effects and failures within networks, and the power outage impact on customers. To achieve this goal, the study undertakes

two consecutive steps: the development of a conceptual framework and of a modelling framework. The conceptualization of flood damage to power grids derives from a thorough literature review. The conceptual framework highlights: (i) the different kinds of damage (i.e., direct, indirect, and systemic) the network can suffer, (ii) the hazard, exposure, and vulnerability parameters on which they depend, (iii) the spatial and temporal scales required for their assessment, (iv) the interconnections between power grids and economic activities, and (v) the different recipients

of economic losses. The development of this framework stresses the importance of dividing the damage assessment into two steps: the estimation of damage in physical units and the consequent economic losses in monetary terms. The variety of damage mechanisms and cascading effects that shape the final damage picture, asks for an interdisciplinary and multi-scale evaluation approach. The literature review reveals the urgent need of combining the available modelling and analysis methods in order to estimate the direct, indirect, and systemic damage to this CI in a coherent manner.

Correspondingly, the modelling framework combines modelling tools and approaches from different disciplines, namely a hydraulic model to generate hazard scenarios, fragility curves to describe the stochastic process of failures of the power grid components, a simulation-based model to analyse the power flow, and a socio-economic model to characterize the customers connected to the power grid. The obtained framework of probabilistic damage assessment allows: (i) considering the magnitude and frequency of floods, (ii)

evaluating the vulnerability of power grids components, (iii) estimating their spatio-temporal probabilities of failure, (iv) analysing the cascading effects across power transmission and distribution networks, and (v) assessing the impact of power outages on the final customers. A synthetic case study is worked out with reference to the IEEE 14 bus system benchmark, which includes the spatial location of the hazard source, of power grid features, and the involved customer categories. The results evidence the propagation of damage to power-dependent economic activities far from the inundated area.

Overall, the conceptual framework provides modelers with an informative tool in support of more comprehensive and reliable flood damage assessments to power grids. Indeed, the use of the modelling and simulation tool, subsequently developed based on the conceptual framework, can enable finding the most critical components for the security of power supply during flooding and its outcomes can assist decision-makers to formulate effective risk mitigation strategies for guaranteeing public security and ensuring financial well-being.

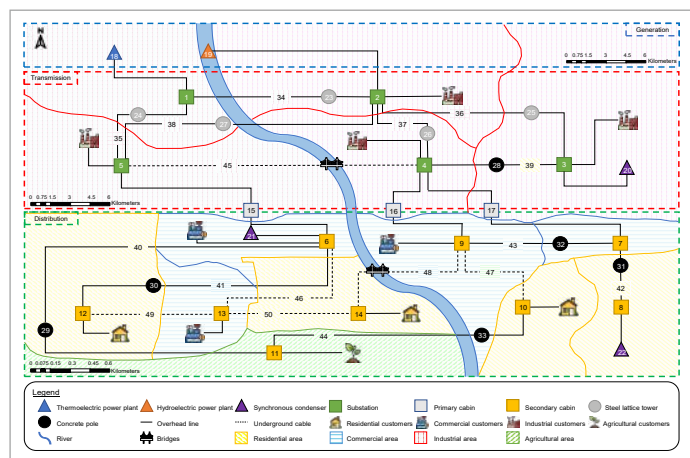


Fig. 1- Sketch of the conceptual representation of the area of interest, crossed by the river (i.e., the hazard source), the power grid systems and components (i.e., generation, transmission, and distribution), and the services areas; yellow polygons represent the residential areas, blue the commercial, red the industrial, and green the agricultural.

## STRATEGIES FOR THE OPTIMIZATION OF RESOURCE RECOVERY FROM SEWAGE SLUDGE ASHES AND OTHER SLUDGE-DERIVED MATRICES TOWARDS PROCESS SCALE-UP

Gaia Boniardi – Supervisors: Prof. Andrea Turolla

Phosphorus (P) is a non-renewable and limited resource commonly extracted from natural phosphate rocks, which are concentrated in non-European countries. Due to the increasing P consumption, mostly addressed to fertilizer manufacturing, and the criticalities related to its supply, both P and phosphate rocks have been introduced in the list of Critical Raw Materials by the European Commission. Among the available P-rich secondary sources, sewage sludge, and derived matrices have drawn increasing attention in the past decades.

At present, the most challenging issues to tackle to recover P from secondary resources are: (i) economic feasibility, (ii) legislation barriers for recycled P, (iii) lack of an established market for recycled products and incentives for the production industry to use them, (iv) lack of detailed technical information about the existing established technologies to support decision making. The main goals of this Ph.D. project are: (i) to optimize the most promising existing technological solutions for P recovery from sewage sludge ashes (downstream of mono-incineration) via wet chemical extraction followed by a dedicated metals decontamination unit and

a subsequent co-precipitation unit, (ii) when incineration is not a viable option, to explore alternative approaches (i.e., wet chemical extraction or biological processes) to extract and precipitate P from other sludge-derived matrices, such as hydrothermal carbonization (HTC) products (i.e., slurry and hydrochar), and activated sludge. The methodology applied comprised laboratory-scale experiments and small pilot-scale experiments combined with the use of modeling and statistical software to optimize the different phases of the P recovery process. A preliminary explorative phase was conducted at lab-scale in which the influence of upstream treatment conditions (i.e., incineration technology and P removal method at the wastewater treatment plant) was investigated. Several ash samples were characterized physically and chemically to identify the main ash characteristics that have a relevant impact on the performance of the P recovery process. Then, two representative samples were selected for the optimization of the P extraction process. Statistical techniques such as Design of Experiments (DoE) and Response Surface Methodology (RSM) were applied to study the effect of several

operating parameters (i.e., acid type and concentration, liquid-to-solid ratio, contact time) on the recovery performances. Optimal extraction conditions identified were successively applied for the tests a small-pilot scale.

To decrease the metal content in the leachate (i.e., liquid obtained after wet chemical extraction) an innovative decontamination strategy was tested using a bio-based adsorbent (i.e., Cellulose Nanostructured Sponges, CNS) synthesized by the chemistry department of Politecnico di Milano. Adsorption tests were conducted in a wide range of pH (1.8–10) and with different CNS dosages (1, 3, and 10 g/L). Then, in the view of circular economy, the co-precipitation of P from the leachate with other nutrients was investigated using a by-product from the mining industry (i.e., low-grade MgO), highly present in Europe, to increase the pH while providing Mg ions for P precipitation.

Results from the wet chemical extraction highlighted the role of ashes properties (e.g., alkalinity) in the extraction process, which inevitably affected the operating costs related to reagents possibly limiting a convenient process scale-up. The optimal settings identified were acid concentration (C)  $C_{H_2SO_4} = 1.3$

N, liquid-to-solid ratio (L/S) = 20, contact time (t)  $t = 2$  h, and  $C_{HCl} = 2.0$  N, L/S = 10,  $t = 2$  h for Ash#1, and  $C_{H_2SO_4}$  or HCl = 0.8 N, L/S = 10 for Ash#2.

The decontamination strategy tested ensured the compliance of the solid precipitate with the European Fertilizer Regulation 2019/1009 when the following conditions were applied: adsorption at pH < 2 with a CNS dosage of  $10 \text{ g}_{CNS}/L_{leachate}$  in the presence of citric acid ( $10 \text{ g}_{citric\ acid}/L_{leachate}$ ), followed by precipitation at pH 8 with  $Ca(OH)_2$ . In detail, the adsorption efficiencies at pH 1.8 for the selected metals (17%, 16%, 11%, 29%, 3%, 38%, and 11% for Zn, Cu, Ni, Cr, As, Fe, and Al, respectively) guaranteed a concentration of these metals in the solid precipitate below the regulatory limits for fertilizers.

Results from the co-precipitation tests highlighted the role of the Aluminum/P molar ratio in the leachate, reporting a satisfactory P Precipitation Efficiency (PPE) when PC8 was used in both lab-scale tests (PPE 68–100%), and small pilot-scale tests (PPE 89–100%). The physical, chemical, and industrial assessment of the solid precipitates obtained from small pilot-scale tests denoted compliance with the EU 2019/1009, which allows the

formulation of different fertilizers with agronomic relevance.

Besides P recovery from sewage sludge ashes, P and carbon recovery from other sludge-derived matrices (i.e., slurry/hydrochar and activated sludge) was explored via wet chemical extraction and acidogenic fermentation (only for activated sludge). HTC products were sampled from a pilot-scale plant, while activated sludge samples were collected during the PhD research period at the University of Queensland from two wastewater treatment plants located in Australia, applying Enhanced Biological P Removal (EBPR) as the main method for P removal. Chemical extraction tests were conducted using two samples of slurry and hydrochar with various acids (including oxalic acid, sulfuric acid, nitric acid, and citric acid) to investigate their impact on metal contamination. The subsequent precipitation stage involved calcium silicate hydrate (CSH), allowing assessment of the fate of heavy metals alongside P during the entire recovery process. For activated sludge samples, acidic extraction was performed with 1 N HCl or  $H_2SO_4$  till pH 2 was reached, while acidogenic fermentation was performed under anaerobic conditions for 24 h without

additional carbon supply. Results demonstrated that oxalic acid was a promising extractant for slurry, while the type of acid used had a lesser impact on hydrochar. The highest Maximum Overall phosphorus Recovery Efficiency (MORE) and the lowest heavy metals/metalloids precipitation were achieved from the hydrochar samples (MORE 74–100%), being the recovery from slurry less effective (MORE 50–75%). The biological process (i.e., acidogenic fermentation) outperformed the chemical extraction from activated sludge in terms of P release when dealing with EBR biomass (P release up to 60%), decreasing the costs of chemical reagents needed. However, the limited overall recovery efficiencies highlighted the need for further research to optimize this process.

## ENVIRONMENTAL ASSESSMENT OF LIME-BASED INNOVATIVE CARBON DIOXIDE REMOVAL AND STORAGE SOLUTIONS

Francesco Pietro Campo – Supervisor: Prof. Stefano Caserini

This PhD work has analysed different atmospheric carbon dioxide removal and storage solutions, assessing their potential environmental and climatic impacts by applying the LCA methodology. All the analysed processes exploit lime for removing or storing CO<sub>2</sub>. Two of the analysed solutions are innovative ocean-based solutions, while the other two, i.e., the lime carbonation and the soil liming, are current lime applications. For limiting the global temperature increase to 1.5°C, an order of magnitude of 100 - 1000 gigatonnes of CO<sub>2</sub> should be removed from the atmosphere during this century. Among the negative emissions technologies, marine carbon dioxide removal (CDR) processes have a high potential, since they are not limited by land availability and the consequent trade-offs related to land use, e.g., arable land competition for food production and energy crop productions. Furthermore, marine CDR such as Ocean Alkalinity Enhancement (OAE), has the co-benefit to counteract ocean acidification, and the CO<sub>2</sub> removed from the atmosphere is stored in the form of bicarbonates in the sea for geologic times of at least 10,000 years.

Enhanced Rock Weathering (ERW) consists of spreading crushed alkaline materials on soils, where atmospheric CO<sub>2</sub> dissolves in soil porewaters in the form of bicarbonates that are drained into surface waters and eventually to the sea. This means that also ERW would store the atmospheric CO<sub>2</sub> as bicarbonates in the oceans. A key aspect related to the present PhD work is that CDR processes require not only removing CO<sub>2</sub> from the atmosphere but also storing it permanently somewhere (e.g., in underground saline aquifers or in the ocean). Both the removal and the storage require energy and materials, so to evaluate the overall climate and environmental benefits it is necessary to consider Life Cycle Assessment (LCA), a standardized methodology often applied to products or processes for evaluating the environmental burdens generated during the life-cycle of a product or a process. After a literature review on LCA applied to CDR processes, the novelty of this study is to apply the LCA methodology to marine carbon dioxide removal and storage solutions, confirming that it is a proper instrument to evaluate the environmental

performance of the removal or the storage. The evaluation of novel solutions for contrasting climate change is essential to have a holistic understanding, to avoid environmental damages or burden shifting and to improve the expected climate benefits. For this purpose, a proper functional unit and a comprehensive system boundary which encloses all phases, i.e., from raw material supply to carbon storage, are essential for meaningful environmental impact assessment, as results from the literature review on LCA applied to CDR processes. The results of this thesis work demonstrate the efficacy and efficiency of a CO<sub>2</sub> removal process based on OAE using three different energy sources for the lime production: renewable electricity, biomass gasification and coal gasification. The largest climatic benefit is achieved in the configuration which combines biomass gasification with limestone calcination, i.e., about 2.4 kg of negative CO<sub>2</sub>eq emission per 1 kg of carbon-free slaked lime used for OAE, that is about 3 times the configuration with renewable electricity calcination. Biomass configuration obtains this high result thanks to CO<sub>2</sub> removed through OAE, but

also thanks to the biogenic CO<sub>2</sub> storage and the avoided impacts due to the hydrogen production surplus. The assessment of the potential environmental burdens in other 15 different categories, in addition to climate change according to the Environmental Footprint method, allows to estimate the potential trade-offs, such as the one between climate change and land use from the configuration that uses biomass as an energy source. As well, the comparison of the different configurations is worthwhile to identify the one which minimizes the environmental impacts, e.g., the configuration exploiting renewable electricity removes a lower amount of CO<sub>2</sub> from the atmosphere than the one exploiting biomass, but requires less land area for its deployment. Moreover, the configuration with coal gasification has higher impacts in all 16 impact categories than the biomass and renewable electricity ones. The amount of CO<sub>2</sub> that can be stored per 1 kg of slaked lime is 0.6 kg, 1.9 kg and 2.4 kg for configurations with renewable electricity, biomass and coal, respectively. Thus, different CO<sub>2</sub> storage techniques are needed as alternative where geological storage is not deployable.

In this work, an innovative CO<sub>2</sub> storage solution, which mimics and accelerates the natural process of limestone weathering and stores CO<sub>2</sub> as bicarbonate ions in the sea. Since this process uses CO<sub>2</sub>, lime and seawater, it suits well with ocean liming. However, in order for this to be efficient, from a LCA point of view, it should be implemented in a decarbonized energy system. For an electricity emission factor (EF) below 25 gCO<sub>2</sub>eq/kWh, similar to the EF of wind (22 gCO<sub>2</sub>eq/kWh) and photovoltaic (17 gCO<sub>2</sub>eq/kWh) calculated from Ecoinvent database, storage efficiencies above 90% are achieved, i.e., the life-cycle GHG emissions are less than 10% of the CO<sub>2</sub> stored. The interest in assessing the potential carbon storage or removal of lime is growing. From the analysis of the current EU lime market presented in this thesis, the storage of CO<sub>2</sub> is about 23-33% of the lime process emissions through the mineralization, in this case the lime carbonation during the use phase of the lime. The time required for the carbonation reaction is instantaneous for three applications of lime, namely in wastewater treatment, in flue gas cleaning and in pulp and paper production. Up to 22% of

the CO<sub>2</sub> calcination emissions are absorbed within five years, based on the current EU market for lime. Furthermore, the future LCA application on soil liming as ERW taking into account the preliminary results presented in this thesis will be essential to understand the potential co-benefits, such as GHG emissions reductions. From the results of the reviewed 30 experimental studies in Europe, soil liming of acid soils increases the soil pH by +30±3%, improving the plant growth and consequently the rise of the crop yield by +90±24%. Moreover, liming treated soils reduce N<sub>2</sub>O emissions compared to non-treated ones, compensating the CO<sub>2</sub> emission due to the soil respiration net of GHG removal from the atmosphere through SOC stock increase and upland CH<sub>4</sub> uptake.

## MODELING HYDROLOGICAL EXTREME EVENTS WITH MULTIPLE DATA SOURCES AND INVESTIGATING THEIR COMPOUND BEHAVIOR

Greta Cazzaniga – Supervisor: Prof. Carlo De Michele

Floods and droughts are extreme hydrological events generated by a combination of several hydro-meteorological and climatic processes across multiple spatial and temporal scales.

Such a combination of processes, leading to significant impacts is referred to as compound event.

In the past, traditional studies on EHEs, such as univariate flood frequency analyses, have been foundational for hydrological risk assessment. However, they focused on individual factors and this did not allow them to capture the complexity of the interconnected processes. Shifting towards a compound perspective represents a profound change in approaching these events.

It allows us to enable more informed decisions for disaster management, climate adaptation, and environmental protection. Our objective with this essay is to gain new insights and implement new methodologies to improve our understanding of EHEs, specifically floods and droughts, also investigating their compound behavior.

We hence present three case studies, dealing with three typologies of compound events, namely temporal, multivariate, and spatial compound events. The first analysis focuses on

temporal clusters of floods, identified as temporal compound events. The objective is to enhance flood frequency analysis and offer insights for flood hydrograph design. The study includes catchments from four flow regimes within the Po basin, Italy's largest basin. Our findings reveal significantly different distributions in flood peak, volume, and duration between clustered (multiple peaks) and single-peak flood events.

We identify the underlying mechanisms driving these differences, pointing out the importance of employing mixture models for modeling flood-related random variables. For practical design considerations, utilizing a mixture distribution also proves valuable, allowing estimation of the likelihood of a quantile being single-peak or multi-peak. Eventually, we observe a correlation between double-peak hydrograph shape and water catchment characteristics, specifically flow regime and size. In the second analysis, we employ a copula-based methodology for flood design. This approach models the multivariate behavior of floods, specifically capturing the dependence between flood volume and peak. We focus on three Italian dams, assessing

their response to hydrological forcings, that are flood events. The primary objective is to evaluate the adequacy of spillways, crucial for ensuring hydrological safety against overtopping. We then compare the dam's response under three assumptions regarding flood-peak and volume dependence: independence, observed dependence, and complete dependence. This comparison highlights the impact on risk estimates when neglecting the consideration of multivariate compound behavior. The third analyzed compound event is the spatial one with a focus on droughts, which often exhibit spatial dependence. We analyze the 2021–2023 European drought, unprecedented in terms of intensity, spatial extent, and duration, and impacting a wide portion of European countries. We perform an attribution analysis, relying on circulation and impact analogs using reanalysis data. We dynamically reconstruct phenomena and their widespread implications. Eventually, for implementing robust analyses on hydrological extremes we need to rely on accurate rainfall data sources, as rainfall is the main downward facing of the water cycle. We hence develop a feasibility

analysis on opportunistic rainfall sensors to check whether they could be a support in the modeling of hydrological extremes. We validate CML-based rainfall estimates in a mountainous and a peri-urban region in Italy and we evaluate their potential in hydrological modeling. Despite the challenges, our findings demonstrate that CML-based data can effectively support hydrological extremes modeling, performing comparably to rain gauges.

# OCEAN LIMING AS A CARBON DIOXIDE REMOVAL TECHNOLOGY: POTENTIAL, LIMITATIONS AND ENVIRONMENTAL IMPACTS

Serena De Marco – Supervisor: Prof. Stefano Caserini

Reaching net-zero CO<sub>2</sub> emissions requires not only sharp and immediate reductions of emissions but also implementation of multiple carbon dioxide removal technologies (CDR) to balance residuals. Mineral-based CDR technologies such as Ocean Liming (OL) and Enhanced Weathering (EW) consist of spreading alkaline substances onto seawater or land to accelerate the natural CO<sub>2</sub> absorptions continuously performed by oceans or soils but at geological timescales. Limestone and mafic rocks are the best raw material candidates due to fast-weathering rates of limestone by-products (e.g., calcium hydroxide) and olivine. To date, an open question is whether the cost and energy requirement to extract and process large amounts of CDR relevant materials may hinder the future widespread development of such approaches. This work embraced the challenge of defining these requirements, highlighting practical ways to lower them, providing a preliminary energy-cost analysis on the dispersal of calcium hydroxide on board a fleet of ships. Hence, firstly, an in-depth literature review on surface mining, comminution

and long-haul transportation of limestone and mafic rocks has been made to elucidate technical challenges, cost, energy demand and energy-saving strategies. Afterwards, calculations on the energy-saving potential and the alkaline dispersal into seawater have been done. The results show that the main energy-intensive activities are material handling and hauling in quarrying, fine and ultrafine grinding, long-haul transportation on road. Based on the data collected, the total average energy demands are 2.5 kWh/t and 4 kWh/t to extract limestone and mafic rocks respectively,

131 kWh/t and 342 kWh/t to mill limestone and mafic rocks down to 18 μm and 14 μm respectively, 86 kWh/t to transport limestone or mafic rocks indistinctly over 100 km. Hence, among all, grinding is the most crucial stage since the energy demand steeply increases with the reduction of the target grain size (Fig 1). Nevertheless, the energy-saving opportunity is considerable, especially in grinding, if investments in advanced technologies and best practices were sustained. The total potential would be 688 TWh/yr if each operation along the mine-to-mill process chain of limestone

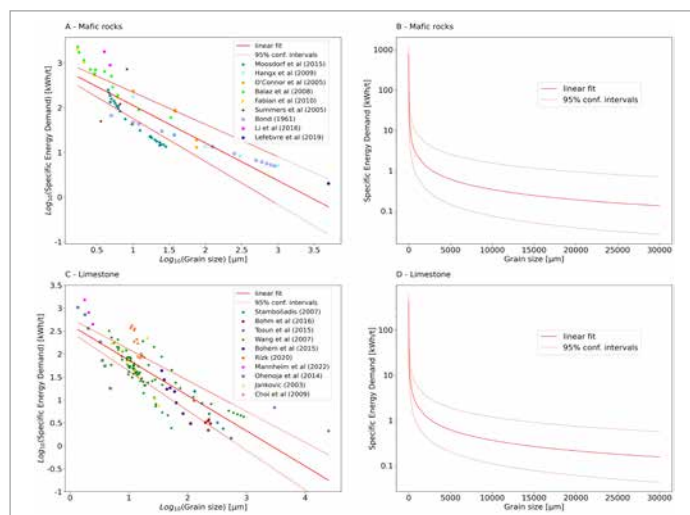


Fig. 1 - Relationships between the energy demand of comminution and the target grain size, in logarithm form (right side, A and C) and polynomial form (left side, B and D) of mafic rocks and limestone.

and olivine was carried out at its own practical minimum of energy; in detail, the sole implementation of best practices could save 296 TWh/yr, whereas implementing energy-efficient technologies from R&D would bring an additional 392 TWh/yr. In a climate change perspective, applying energy-saving strategies to mill limestone and basalt down to 5 μm for OL and EW purposes in the near-medium term (2025-2050), would reduce the electricity demand and the operating cost by 56%-65% in an optimistic scenario (i.e., carbon removal target up to 50 MtC/yr, high economic growth and low zero-carbon technology cost), and, by 43%-51% in a pessimistic scenario (i.e., carbon removal target up to 27 MtC/yr, low economic growth and high zero-carbon technology cost)(Fig. 2). The energy and cost requirement of spreading Ca(OH)<sub>2</sub> into

seawater by using fleets of existing ships is influenced by the alkaline concentration and the discharge rate. The dispersal in form of alkaline solution at low concentration (<1 g/L) can reduce the impact on the marine environment but requires higher water amounts, energy, and cost. A slurry is less costly but a yearly removal of 1 tonne of CO<sub>2</sub> at 10 \$/tCO<sub>2</sub> needs a yearly discharge of at least 1.2 Gt of Ca(OH)<sub>2</sub> at 50 kg/s per trip and around 1,000 bulk carriers of 75,000 dwt each. Complementary to CDR, a techno-economic analysis of a novel carbon capture and storage option called Buffered Enhanced Weathering of Limestone (BAWL) has been proposed. The novelty of BAWL is that CO<sub>2</sub> coming from an industrial source (e.g., Steam Methane Reformer -SMR, calcination) can be converted into an ionic solution and safely discharged in deep

seawater to support the buffering capacity of oceans with minimal risk of CO<sub>2</sub> degassing. This is achieved by mixing CO<sub>2</sub> with calcium carbonate and seawater within a long pipeline called dissolution reactor and buffering the remaining unreacted CO<sub>2</sub> at the end of this reactor with a second mixture of Ca(OH)<sub>2</sub> and seawater. The electricity consumption and cost to store 1 tonne of CO<sub>2</sub> from SMR range from 1.3 MWh to 2.2 MWh and from 142 € to 189 € depending on the combination of three design parameters: discharge depth (100-3,000 m), length of pipeline (10-100 km), grain size of calcium carbonate (10-1 μm). A recent evolution consists of mixing Ca(OH)<sub>2</sub> and CO<sub>2</sub> within one, shorter pipeline (2 km), discharging the buffered solution at 20 m and using a grain size of 74 μm. The energy and cost demands are 214 GWh/tSMRCo<sub>2</sub> and 159 €/tSMRCo<sub>2</sub> respectively.

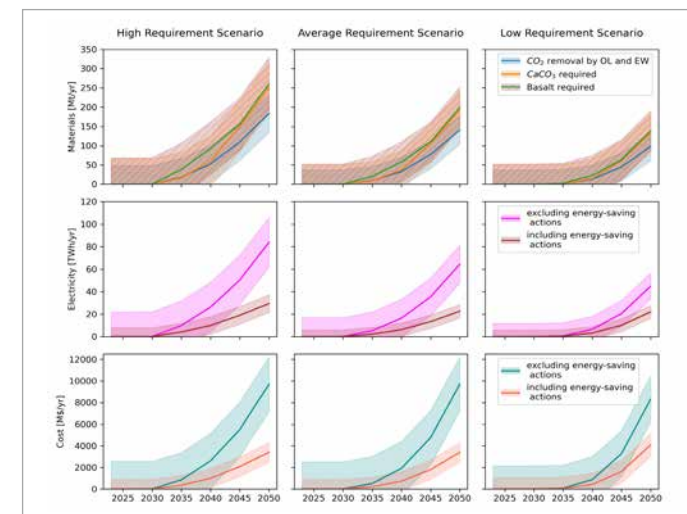


Fig. 2 - Future amounts of CO<sub>2</sub> removal from the atmosphere by OL and EW, CaCO<sub>3</sub>, basalt (top), electricity to comminute limestone and basalt (P<sub>80</sub> = 5 μm) (middle) and cost (bottom), including and excluding energy-saving actions and depending on the scenario. Shaded areas represent 95% confident intervals.

# MICROBIOLOGICAL WATER QUALITY IN DRINKING WATER DISTRIBUTION SYSTEMS: FROM MONITORING TO MANAGEMENT

Marco Gabrielli - Supervisor: Prof. Manuela Antonelli

The importance of monitoring drinking water distribution systems (DWDSs) has been stressed in recent regulations due to their relevance for the quality of drinking water at the consumers' taps. Besides possible intrusions and chemical leaching from pipes, microbial communities within DWDSs have been linked to potential public health issues (i.e., favoring pathogens survival), management (i.e., biocorrosion) and organoleptic (i.e., taste&odor compounds) nuisances. Current monitoring practices are limited by DWDSs complexity, the lack of data and intrinsic uncertainties. Given this difficulty, the degree of microbiological variability in both space and time is not yet well characterized. However, as several regulations rely on the concept of "no abnormal changes", a clear understanding of these variations and their relevance for public health and DWDSs operations is needed. In addition, to further improve DWDSs management, a clearer understanding of their microbiome is critical. In fact, while drinking water monitoring campaigns usually focus exclusively on bacteria, also archaea, eukaryotes and viruses are present and play a role in shaping water quality both with

respect to its microbiological and chemical quality.

The goal of this PhD project is to contribute to the understanding of DWDSs microbiology, improving strategies to design monitoring campaigns and the understanding of the DWDSs microbiome and its spatio-temporal variability. Within this framework, sampling campaigns, simulations and literature data were used to (i) describe microbiological and microbiologically-related water quality variability in DWDSs, (ii) characterize the members of the DWDSs microbiome, and (iii) test monitoring strategies aimed to capture such variability with minimum information requirements.

Firstly, a new procedure for the evaluation of the performance of monitoring locations within DWDSs (i.e. the ability to detect an alteration of the water quality) has been developed to take into account the impact of water demand variability and to focus predominantly on the most impacting water quality alteration events thanks to an initial hydraulic-based importance assessment and the generation of synthetic water demands. Comparisons with traditional strategies highlighted how the most impacting events, despite being detected more easily and in less time, were still linked with higher consumption of altered water. Not accounting water demand variability led to an overestimation of the detection likelihood. In addition, the results showed the importance of

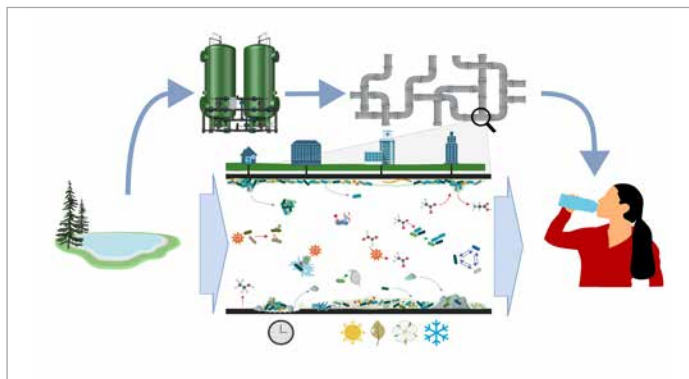


Fig. 1 - Schematic representation of DWDSs and the microbial processes occurring within them.

dilution and minimum detectable concentrations on the expected performances. This procedure was applied to 12 DWDSs where monitoring locations were selected using graph-based methods. This dataset was, first, used to understand the role of topology in quality alterations detection. Secondly, the data was used to identify the best graph-based methods as a function of DWDS topology and the number of monitoring locations selected. The performance of the methods selected was validated using an additional DWDS.

Secondly, two algorithms were developed to automatically optimize sampling times to target daily maximum concentrations or maximum concentration variations. Their performances were compared to traditional schemes using two synthetic scenarios and real-world data. The two algorithms, relying on the multi-armed bandit framework, provided a more accurate representation of the target concentrations with a lower number of samples than traditional schemes. Only having prior information led one traditional strategy to achieve better performances than the two algorithms, highlighting their applicability when no previous information is available. Finally, practical guidance to aid the adoption of these algorithms was provided.

To characterize the temporal variability of the microbiological quality within DWDSs, a monitoring campaign was

performed in a non-chlorinated system for 5 months using online flow cytometry and plate culturing. Analysis of the cytometric fingerprints allowed to detect daily and seasonal variations both in the cells' concentration and in the phenotypical characteristics of microbial communities which were linked to fluctuations in local water demands and chemical-physical water quality. In the absence of notable seasonal variations, daily fluctuations in both concentrations and microbial communities were comparable to those occurring across multiple weeks and showed reproducible patterns. Plate cultures allowed to detect less than 1% of the total cells, not allowing to properly discern the patterns observed by flow cytometry. Finally, different scenarios, simulating different monitoring campaigns, were obtained from the flow cytometry data, assessing the impact of monitoring choices on the variability observable and providing guidance for future campaigns.

To better characterize DWDSs microbiomes and facilitate the analysis of the eukaryotes present, a benchmark of the tools used for eukaryotic-focused metagenomics was performed, leading to the development of a dedicated workflow named EUKsemble and in guidelines for eukaryotic genome reconstruction. This workflow was applied to the metagenomes derived from 81 DWDSs. The analysis of this data highlighted

generally low (i.e., < 1%) eukaryotic content, indicating an under-representation in current data. Nonetheless, their relative abundance was affected both by source water type and residual disinfectant concentrations. In addition, positive correlations between the  $\alpha$ - and  $\beta$ -diversity of eukaryotes, prokaryotes (i.e., bacteria and archaea) and viruses highlighted the effect of current management strategies on the entire microbiome. Finally, the effect of disinfection strategies, source water type and climate on their detection in DWDSs was estimated for several groups of co-occurring eukaryotic taxa.

Finally, the effect of drinking water distribution on chemical water quality was assessed thanks to a monitoring campaign spanning multiple locations within a nonchlorinated DWDS over a whole year. Natural organic matter (NOM) characteristics, estimated through PARAFAC analysis of fluorescence data and absorbance indexes, highlighted the variability of groundwater sources and the different fate during treatment of distinct NOM fractions. Within the DWDS NOM characteristics were primarily shaped by the treatment plants outlets, even though local variations suggested the importance of the "last meter" before the consumers' taps. In addition, our results stress the need to experimentally validate water sources using conservative parameters which could highlight differences with the hydraulic behavior predicted by hydraulic models.

## REDEFINING LIVESTOCK SUSTAINABILITY: TAKE ACTION ON ANIMAL FEEDING TO AVOID RESOURCE-DEPLETING FARMING SYSTEMS

**Camilla Govoni** - Supervisor: Prof. Maria Cristina Rulli

The extent to which livestock production competes directly or indirectly with food crops has often been central to the discussion on environmentally sustainable dietary choices and food security. While animal foods contribute to the global food supply and are an important protein source in human diets, their production uses a disproportionately large fraction of agricultural land and water resources. Therefore, a global comprehensive understanding of the extent to which the livestock sector currently requires valuable natural resources is needed. Then, once it has been proved that livestock feed is made up of a significant amount of human-edible ingredients, such as grains and soybeans, and that the associated use of natural resources could make livestock farming unsustainable, especially in light of population growth projections, new sustainable strategies are investigated. Agricultural by-products, former foodstuffs, and insect meals have been evaluated as potential alternative feed ingredients since their (re)use in animal diets seems to be one of the most sustainable strategies to meet the growing feed demand by using fewer resources while

reducing competition. The results highlight that both land and water savings could be achieved domestically, while a reduction in the virtual land and water trade would allow for greater availability of resources at the local level, lower dependence on imports for some countries, and curbing global environmental issues such as deforestation, GHG emissions, biodiversity losses, and water scarcity. Given these large environmental benefits, the findings incentivize feed researchers and producers to further explore the food safety of this strategy and its implementation to make the food system more sustainable. However, while the use of low-impact feed ingredients can reduce the rate of natural resource consumption and cross-sectoral competition, an effort to decrease animal source food consumption has to be carried on, as suggested by the EAT-Lancet recommendations, since it remains the most effective strategy in this regard.

# REACTIVE TRANSPORT MODELLING OF A CHLORINATED SOLVENTS PLUME AND UNCERTAINTY ANALYSIS: A CASE STUDY

Pietro Mazzon - Supervisor: Prof. Luca Alberti

The contamination of groundwater is a worldwide problem, since groundwater constitutes a large part of the freshwater resource worldwide. Among all pollutants, chlorinated solvents are widely dispersed and most difficult to remove since they are denser than water. Different remediation techniques have been developed over time, but major developments are being made in bioremediation technologies, that involve the use of organisms to degrade the target contaminants. Bioremediation is becoming more popular thanks to its proven efficiency, its relatively low cost, the resulting complete conversion to non-toxic compounds (if correctly handled) and the safety of operators during the remediation activities (little material handling and exposure). However not all sites are suitable for bioremediation. Site specific characteristics such as low permeability or highly heterogeneous materials, the presence of free product, or fractured bedrock sites, can hinder bioremediation. Furthermore, bioremediation can be slower than other techniques (e.g., thermal, or chemical technologies), an aspect that should be considered as well. To test the site suitability for

bioremediation, it is useful to follow several lines of evidence. The past reduction of concentration over time and space (plume shrinking), suitable geochemical conditions (e.g., anaerobic environment), presence of microorganisms and biomarkers and occurrence of isotope fractionation are examples of such evidence. A tool that can be used to evaluate and extend the lines of evidence grows out of the development of a groundwater flow and transport model. Models are useful to include different field information in a single framework, which is also able to make predictions (once calibrated) that can be compared in different scenarios, also considering the uncertainty of parameters and results. As an example of possible application of bioremediation technologies, the present thesis

work evaluated biological-based solutions for the management of a chlorinated solvents contamination in a former industrial site located in southern Italy, where TCE, cis-DCE and VC are present in groundwater. Specifically, the application of Monitored Natural Attenuation was evaluated, relying on the presence of existing attenuation mechanisms at the site. First, a statistical analysis was performed on concentration data, identifying a decreasing concentration trend along the flow direction, with very low measured concentration values towards the site boundaries. Then, the Compound-Specific Isotope Analysis (CSIA) data retrieved from an isotopic field survey were analyzed, showing an enrichment of the isotopic composition of the contaminants proceeding downgradient of the source; this

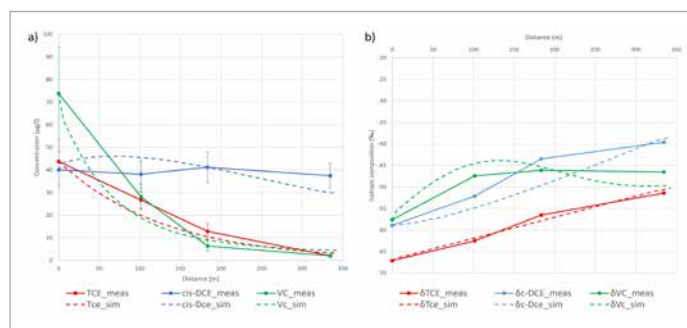


Fig. 1 - Results of 1D reactive transport and isotope fractionation simulation.

behavior is strictly related to biodegradation. Finally, different analytical (BIOCHLOR-ISO) and numerical models (MODFLOW-USG Transport, PHT3D, PHT-USG and others) were developed to test the hypothesis of active biodegradation at the site, employing different codes and progressively increasing the complexity of the models. After calibration, the model results support the hypothesis of active biodegradation mechanisms at the site, looking both at concentrations and isotopic compositions, even considering the uncertainty of parameters and predictions. The modelling tools were then used to test possible remediation strategies for this contamination, considering two scenarios. The model predictions were evaluated under uncertainty to look for the different expected results of

the two scenarios, evidencing pros and cons and estimating the possible remediation time frames. The novelty of this work lies in the application of very recent, powerful codes (such as PHT-USG) and new uncertainty analysis techniques (PESTPP-IES) to Reactive Transport Models, applications that are largely absent from the scientific literature. Furthermore, the simulation of the 2D isotopic composition within the plume is an application not widely studied in literature, but with a great potential for interpretative and predictive purposes. Finally, the document is sort of a guide for similar cases, where bioremediation is an option on the table. Indeed, it demonstrated the usefulness of models in testing the conceptual model and supporting the decision for the

contamination management, also helping in the discussion with the public authorities and supporting the reliability of bioremediation for selection as a remediation technique.

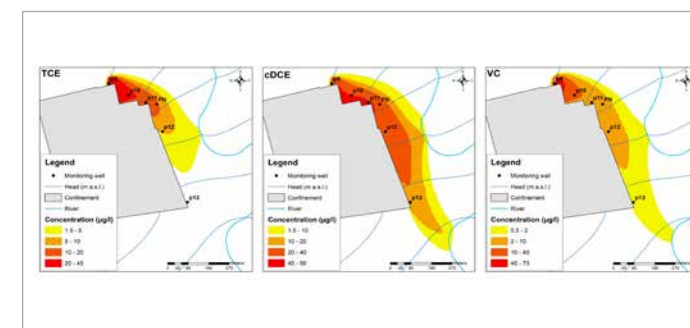


Fig. 2 - Results of 2D reactive transport simulation.

## INVESTIGATION OF DISINFECTION IN DRINKING WATER DISTRIBUTION SYSTEMS

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Recent global guidelines emphasize the importance of ensuring reliable water quality for human health, from both a microbiological and chemical perspective, from source to tap, through a comprehensive risk assessment and management approach of drinking water distribution systems (DWDSs). Chemical disinfection is the last barrier in the water treatment train to ensure microbiological safety of drinking water which is increasingly threatened by climate change. Inefficient chemical disinfection can result in several drawbacks, including altered water organoleptic properties, accelerated pipeline wear, and increased formation of disinfection by-products (DBPs). The recent UE Drinking Water Directive 2022/2184, beside revising water quality standards, posed attention on materials that come into contact with drinking water, with a focus on ensuring compatibility with different water conditions and avoiding leaching of potential compounds that could alter water quality. Despite the attention given to chemical and biological water stability in DWDSs, there is a lack of knowledge about optimizing disinfectant strategies. This includes selecting the most suitable disinfectant, correctly

measuring it, and modelling its behaviour, such as its decay due to water quality conditions and its interaction with pipe materials. These factors make it difficult to plan and manage disinfection processes up to consumers. The aim of this PhD project is to develop strategies to optimize disinfection processes in DWDSs and to investigate and model the behaviour of the two most commonly applied chemical disinfectants, i.e. sodium hypochlorite (NaOCl), which is a chlorine-based disinfectant, and chlorine dioxide ( $\text{ClO}_2$ ). Specifically, the following aspects were investigated: (i) disinfectant measurement, (ii) disinfectant decay as a function of water composition, (iii) interaction between water and pipe material, in terms of both leaching and disinfectant decay, as a function of water quality, type of disinfectant, and pipe material. Laboratory-scale experiments and modelling work were integrated to fill knowledge gaps and to provide solutions for planning disinfection processes that minimize health risks and operational issues. Firstly, different methods for measuring  $\text{ClO}_2$  in stock and diluted water solutions were tuned and compared. In fact, conventional methods, i.e.

iodometric titration for stock solutions and N,N-Di-n-propyl-1,4-phenylenediamine (DPD) colorimetric method for diluted solutions (concentrations lower than 1-2 mg/L), are sensitive to the presence of chlorine, hampering the selective determination of  $\text{ClO}_2$ , which is important in complex disinfection systems where multiple disinfectants may coexist. Suitable chlorine masking agents were selected and their proper concentration was identified. In addition, a reliable procedure using the chlorophenol red pigment colorimetric (CRP) method was developed for the selective measurement of low  $\text{ClO}_2$  concentrations. The optimized DPD and CPR methods were compared to determine the best alternative and the CPR method was found to be the most appropriate. Chlorine-based disinfectants are the most widely adopted and a lot of research studies can be found describing their decay in water as a function of water quality. However, this huge amount of information is hard to be compared, since it is highly case-study sensitive, and then used to properly manage disinfection in the DWDSs. In this PhD project, a meta-analysis approach was adopted to generalize the

estimation of coefficients for three types of chlorine decay kinetic models (first-order, second-order and two-reactants). Literature data were collected and statistically processed to develop empirical models to predict decay coefficients based on water quality and disinfection operating conditions, overcoming the site-specificity of the original models. The effectiveness of the developed empirical models was tested against literature data. The two-reactants kinetics was found to be too complex to provide reliable estimates, while the developed empirical models for first-order and second-order kinetics resulted to be useful tools for predicting chlorine decay in the absence of field data and in different case scenarios. Finally, the interactions between water quality, disinfectants (no disinfectant, NaOCl, and  $\text{ClO}_2$ ), and pipe materials were investigated focusing on two different materials, which are typical of big (cement-mortar lined pipes) and small (cross-linked polyethylene pipes) pipe diameters. The migration from cement mortar-lined pipes as a function of water aggressivity and disinfectant conditions was investigated through laboratory batch tests. In particular, a new testing protocol was proposed

to consider disinfectant decay and pipe ageing. Results stressed that, in case of new pipes, NaOCl rapidly decays and reacts with the organic compounds leached by additives contained in the cement-mortar lining, potentially forming harmful DBPs. However, in the case of aged pipes, both for NaOCl and  $\text{ClO}_2$ , disinfectant decay due to the reaction with cement mortar lining became negligible. Water characterized by high aggressivity caused greater leaching leading to an increase in water hardness and disinfectant decay rate with respect to water with lower aggressivity. As for cross-linked polyethylene pipes (PE-X), three types of materials were selected (PE-Xa, PE-Xb and PE-Xc) and used in laboratory batch experiments. Tests using PE-X in powder form were performed to evaluate the maximum potential release of organics and formation of DBPs. To identify the source of organics release, an antioxidant (Irganox 1010) frequently used in PE-X pipe manufacturing was tested as pure compound. Disinfectant decay, organic carbon characterization and leaching of volatile and semi-volatile compounds in water were evaluated, also using non-target screening analyses to obtain a complete overview of the compounds that could

leach from the pipes and to conduct a preliminary health risk assessment. It should be stressed that, on average, more than half of the released compounds were not found in compounds libraries. In almost all cases, a greater extent of release was observed for  $\text{ClO}_2$  disinfection, due to its high reactivity compared with NaOCl, although different types of analyses provided non homogenous results and further research is needed.

## DEVELOPMENT AND APPLICATION OF A MULTI-SCALE MODELLING SYSTEM FOR AIR QUALITY MANAGEMENT IN URBAN AREAS

**Andrea Piccoli** – Supervisor: Prof. Giovanni Lonati

Air quality is considered one of the main environmental risks for urban areas. Considering that most of the global population resides in urban areas and that this share is expected to keep growing in the coming years, strategies to reduce atmospheric pollution should be a pressing concern for policy makers. In 2021 the World Health Organization (WHO) updated their air quality guideline values for the protection of human health, reducing the thresholds of acceptable concentration for most pollutants analysed in the study. For this reason, the European Commission recently proposed a revision of the current European Air Quality Directive with stricter reference values to better align the regulatory limits with the WHO values. The road transport sector is the biggest emitter of NO<sub>x</sub> and fourth for PM<sub>10</sub> emission in the European Union. Especially in urban areas, where other sources as industry and agriculture are low, the role of road traffic is even more important. Consequently, several municipalities placed limits on circulation of the most polluting vehicles by introducing Low Emission Zones (LEZ). A newer development, still experimented by few cities, is the introduction of Zero Emission

Zones (ZEZ), defined as areas where only vehicles of zero tailpipe emissions are allowed to circulate. Milan, a city in northern Italy, is among the C40 Cities Climate Leadership Group global network that pledged to have a zero emission area within the city by 2030. Air quality modelling studies are the most promising tools to evaluate the potential impacts of planned measures on mobility, also including the establishment of LEZs and ZEZs. The general goal of this thesis was to develop a modelling chain to evaluate the effects of clean mobility on air quality and human health. To this aim, a four-module modelling chain was set up and tested for the city of Milan. The thesis project was divided into three main parts: the first two were focused on the development of the modelling chain; the third part was dedicated to its application over the city of Milan. In the first section of this thesis the set-up of the main structure of the modelling chain is presented. The first module of the chain estimates the average daily traffic for both public and private transport in the city of Milan. For the private sector a road traffic model was used to compute the circulating number of vehicles for each road link, while public transport

traffic was calculated starting from open data of bus lines and timetables. The following step was the bottom-up estimation of road traffic emissions using the HERMESv3\_BU model. Dedicated preprocessing scripts were created to link the traffic data with the emission model and to connect the simulated emission fields the Eulerian air quality model CAMx, which represents the third module of the modelling chain. Along with the traffic emissions, with the Eulerian chemistry and transport model we also simulated the emissions of all other sectors, estimated through the classical top-down emission inventories. Air quality simulations were carried out using a set of two nested domains: the outermost domain covers the entire Italian peninsula with a 4-km horizontal resolution and a 1-km nested domain is centred on the city of Milan. Finally, the fourth module estimates the long-term impact on human health of NO<sub>2</sub> and PM<sub>2.5</sub> following the latest WHO recommendations. The added value of the modelling chain is evaluated by comparing the simulation results for NO<sub>2</sub> and particulate matter ambient concentrations with those obtained with the classic top-down approach and with

observed data. Simulation results show improvements in the accuracy of model predictions over the urban area and highlight the importance of properly accounting for dust resuspension in traffic policy evaluations because of its increasing contribution to PM traffic emissions in the future. In the second section, the enhancement of the Eulerian air quality model to a hybrid Eulerian-Lagrangian model is presented and tested. Such enhancement is obtained through the Linear Plume in Grid (LPiG) module, a Lagrangian model online with CAMx, with the goal of simulating the dispersion of road traffic emission at the sub-grid scale. LPiG is developed by extending the Lagrangian puff sub-grid PiG (Plume in Grid) model already available in CAMx. The online pairing of the local scale Lagrangian model with the regional scale Eulerian model eliminates the problem of the double counting of emissions, leading to a multiscale simulation of air quality from the regional scale to the urban scale. The new hybrid model is evaluated for NO<sub>2</sub> in the city of Milan, showing improved performance compared to the classical Eulerian approach. Finally, the third section of the

thesis presents the simulation of a clean mobility scenario for Milan. This scenario simulation takes advantage of all the developments introduced in the modelling chain for the better evaluation of road traffic emissions and dispersion in the urban area. Additionally, the scenario analysis also calculates the impacts on human health of the transition to a cleaner mobility, a useful piece of information to better communicate the possible advantages of the improvement in the air quality levels to a wide public. Here, we analysed two scenarios: the baseline evolution of emissions to 2030 as planned by the European regulations (BAS30) and the implementation of ZEZ in Milan city centre in the 2030 emission context (ZEZ30). The impact of the policy is inferred by comparing results for BAS30 and ZEZ30 scenario with the baseline simulation for 2017 (BAS17). A strong reduction in road traffic emission is expected for the BAS30 scenario in the city of Milan that, along with the emission reductions of the other sectors, will lead to a projected reduction in ambient concentration for the city of Milan compared with the year 2017 of 54% and 35% for NO<sub>2</sub> and PM<sub>2.5</sub> respectively.

Consequently, morbidity and mortality indicators are expected to decrease of 50% circa in 2030 scenario compared with the BAS17 simulation. The ZEZ in Milan city centre is expected to strongly reduce the road traffic emissions, but its effect on air quality is limited given the small area covered by the ZEZ and the already strong concentration reduction simulated for the BAS30 scenario. The hybrid modelling chain with the bottom-up assessment of road traffic emissions proves to be an effective tool to analyse the impacts of mobility policies on air quality and human health. While in this thesis the city of Milan was used as the test case to validate and test the modelling set up, the modelling chain can be easily applied to other locations where traffic data information is available.

# AERODYNAMIC NOISE GENERATION BY PERFORATED PLATES IN DUCTS

Luca Nicola Quaroni - Supervisor: Prof. Stefano Malvasi

Co-Supervisor: Prof. Islam Ramadan

The fact that air flows generate sound under specific conditions has been known to humans from time immemorial, as the use of wind instruments in prehistoric societies testifies. However, it is not until the 1950s that scientific theories have been developed to study the mechanisms behind such phenomenon. This is because the issue of generating high levels of aero-dynamic noise rose in importance only after the introduction of jet engines in commercial aircrafts, prompting engineers to find solutions for its reduction.

While developed principally in the field of aviation, the problem of aero-dynamic generation of noise is by no means limited to such domain. In many fluid-dynamic processes in fact, there is the need to perform some sort of flow rate control. In pipe and duct systems, this is usually done through the use of valves, which come under many different shapes and formats. Their basic mechanism is to cause localized energy losses through flow constrictions so as to dissipate excess energy. This allows in turn to decrease the flow rate that the flow is able to convey. The majority of the energy is dissipated to heat through viscosity. However, a

small part of it is converted into sound. The generated acoustic pressure waves then travel along the system and are transmitted to the outside environment through the vibrations of the ducts' walls. Due to the particular way in which acoustic waves propagate in closed systems (with non-homogeneous distributions over the cross-section known as higher-order modes), the internal flow geometry of the flow control device (e.g. valve) may selectively enhance or hinder sound propagation for a given frequency range. Furthermore, for the case of pipes, such higher-order modes contribute particularly to the noise transmitted to the outside environment.

A better understanding of the influence of the valve geometry on the generated acoustic field within the pipe/duct may hence permit the development

of devices which mitigate sound production and/or its transmission to the outside environment.

The present work is an attempt to gain a more robust knowledge of the effects of a flow control device's geometry on its broadband aerodynamic noise generation. Due to the large variety of flow control devices available, it has been chosen to focus on the case of perforated plates. Such devices in fact display the same basic phenomena found in more complicated ones (e.g., flow constriction, noise generation) while keeping the geometry simpler and more amenable to a deeper analysis of the governing geometrical parameters.

The approach followed in the thesis is a blend of theoretical and experimental work: the available theory on the subject is

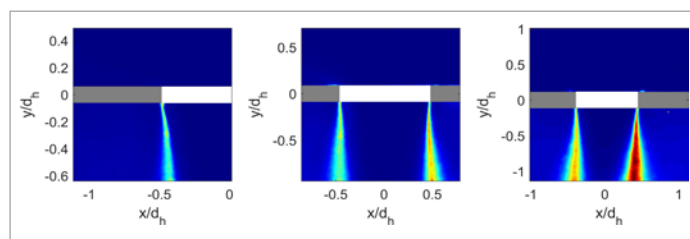


Fig. 1 - Normalized mean turbulence kinetic energy field for different rectangular plates tested at a low-speed facility through Particle Image Velocimetry techniques. Values range from 1 (dark red) to 0 (dark blue). Solid surface is represented in gray and orifice's position in white.

used as guidance in the choice of the parameters most probably affecting noise generation.

Experiments are then performed to validate the theoretical findings and to provide a useful reference for additional works on the topic. In particular, two air flow conditions have been considered in the analysis. Firstly, the case for which compressibility effects are negligible due to the low velocities within the flow when compared to the speed of sound in the fluid. Such condition is common in Heating, Ventilation and Air Conditioning (HVAC) systems and will be referred to in the following as 'incompressible flow' (it has to be highlighted here that such a definition relates to the fluid-dynamic behaviour of the flow, and not to the acoustic one). Secondly, the case for which compressibility effects are important but where the maximum local velocity is anyway less than the local speed of sound. Such case is common in the Oil & Gas (O&G) industry, where control valves usually operate up to the point where sonic conditions are

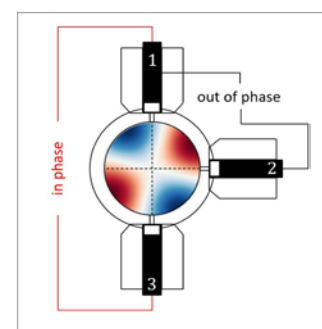


Fig. 2 - Schematic representation of non-uniform distribution of acoustic pressure fluctuations in the instrumented cross-section of a newly set-up experimental plant at Politecnico di Milano.

reached. In the following, such flow regime will be referred to as 'subsonic flow'.

The present work provides some original contributions to the body of knowledge on the topic of broadband noise generation by flow through perforated plates. In particular, it is shown that, at least in the incompressible flow range, the modal content (in terms of higher-order acoustic modes) of the generated broadband noise can be modified through a choice of the position/number of the orifices in a perforated plate. A qualitative 'modal efficiency coefficient' for a preliminary characterization of the aptitude of a given orifice geometry in exciting a specific higher order mode is derived based on considerations on the available knowledge from the literature.

An experimental campaign in a low Mach number test facility allows to validate this theoretical finding by estimation of the higher-order modal components of the emitted acoustic power for different orifice dispositions in a rectangular plate. Experiments included a particle image velocimetry measurement campaign for the visualization of the near-field average flow behaviour upstream and downstream of the orifice plates. It was found that the orifices' number and positions greatly influence the acoustic emissions while the flow pressure drop caused by the obstacles is similar. The proposed qualitative 'modal efficiency coefficient' showed good agreement with the experimental results.

To test whether this was limited to incompressible flows only, a second experimental campaign was performed on a new test bench allowing for up to sonic conditions to be reached in the flow *vena contracta*. The validation of the newly-setup plant at the 'G. Fantoli' Hydraulics' Laboratory of Politecnico di Milano is described and the results of tests on perforated plates with different combinations of orifices' number, disposition and thickness are reported. Due to the presence of whistling for most of the geometries, no general remarks could be made on the influence of such parameters on broadband noise generation. However, the importance of the higher-order modes in the only case for which no whistling was detected is highlighted by coherence estimates of the wall pipe pressure fluctuations measured by sensor pairs at the same cross-section, far downstream of the perforated plate under test.

## ENVIRONMENTAL SUSTAINABILITY LIMITS TO VEGETATION EXPANSION

**Livia Ricciardi** – Supervisor: Prof. Maria Cristina Rulli

Water is the essence of life on Earth since it is needed in every human activity (e.g., agriculture, industry, domestic use). Currently, the demand for water is ever increasing following different human pressures, therefore sparking competition among different water uses (e.g., food, cash crops, and energy production). Among these, the food system does not only overexploit the environment but also reflects food habits detrimental to human health. To date, to meet the demand for food and other commodities, humans have progressively encroached into ecosystems by both expanding agricultural production in wildlands and by intensifying current agricultural production. However, the extent to which it is possible to fulfill human needs while ensuring sustainability for both humans and the planet (e.g., water resources use) is still unclear. To close this literature gap, this doctoral dissertation explores the environmental limits to sustainable expansion of agriculture (and agroforestry) and to crop replacement strategies by using spatially distributed hydrological and land allocation models. In particular, this work first investigates whether enough water is

available to allow expansion in wildlands for producing cash crops. The same procedure is used to assess whether it is environmentally sustainable to plant trees to store carbon dioxide as a climate change mitigation strategy. Then, this thesis investigates the feasibility of expanding food production to cope with trade shocks (e.g., food bans following the Russo-Ukrainian war), as predicted by economic models. This thesis finds that, in most cases, it is not possible to expand agriculture without inducing or exacerbating water scarcity either locally or downstream. In addition, competition for water among all uses would also be aggravated. However, in a particular case study, sustainable agricultural expansion would still be possible when selecting only those areas not inducing water scarcity exacerbation (i.e., in the case of coffee expansion in Kenya). Lastly, this thesis finds that dietary changes towards sustainable diets (i.e., healthy and less water intensive) could be achieved, to a certain extent, through crop replacement both at local and at global scale. Hence, while cropland expansion is at large unsustainable, crop replacement could help achieve water savings. Given

the strong connections between environmental issues and other fields of study, this thesis also covers topics ranging from economic matters to public health targets, using a transdisciplinary approach which could be applied to numerous other case studies.

# PROBABILISTIC STUDY OF FLUID MIGRATION AND ALLOCATION OF UNDERGROUND ENERGY RESOURCES

Rafael Leonardo Sandoval Pabon - Supervisor: Prof. Monica Riva

The main motivation underlying the PhD Thesis is tied to the recognition of the key role that underground resources consistently play in the context of energy production across the globe, this role being particularly relevant during the energy transition era. Even as the field of underground energy resources has attained a high level of maturity, there are still some major barriers limiting our knowledge and ability to effectively quantify and manage environmental impacts of these activities. These barriers are intimately related to the recognition that management of underground systems is challenging due to a variety of reasons, mostly related to uncertainty. The work performed in the PhD consists of (a) fundamental research and (b) rigorous original modeling frameworks that explicitly recognize and effectively deal with ubiquitous uncertainties associated with natural systems. The primary goal of the Thesis is to expand our knowledge on reservoir geosystems with the aim of optimizing the efficiency of underground energy projects as well as to quantify (with the aim of minimizing) environmental side effects of these types of projects whilst considering multiple sources of uncertainty. This is accomplished through a detailed

probabilistic study of three critical aspects of hydrocarbon production. A model to represent gas flow in low permeable materials is analyzed in the first part of the Thesis. The model conceptualizes gas migration as the result of surface diffusion and two weighted bulk flow components, corresponding to slip flow and Knudsen diffusion, whilst considering effects of mechanical deformation, the presence of real gases, and adsorption-desorption dynamics (See Figure 1). Precise description of gas flow in caprocks allows for the quantification of the sealing efficiency of these types of geomaterials. The latter is a necessary step for successful implementation of projects aiming

at storing gases like methane, hydrogen, and carbon dioxide in underground reservoirs. The gas flow model is analyzed via two modern global sensitivity analysis methods. This yields the identification of (i) the parameters with the highest contribution to model predictions uncertainty; (ii) the input-output relationship between model parameters and model predictions; and (iii) the flow mechanism with the largest contribution to the overall gas flow under typical caprock conditions as well as its precise contribution to the overall flow dynamics. Potential effects of hydraulic fracturing activities on groundwater bodies are analyzed in the second part of the Thesis. These types of activities are

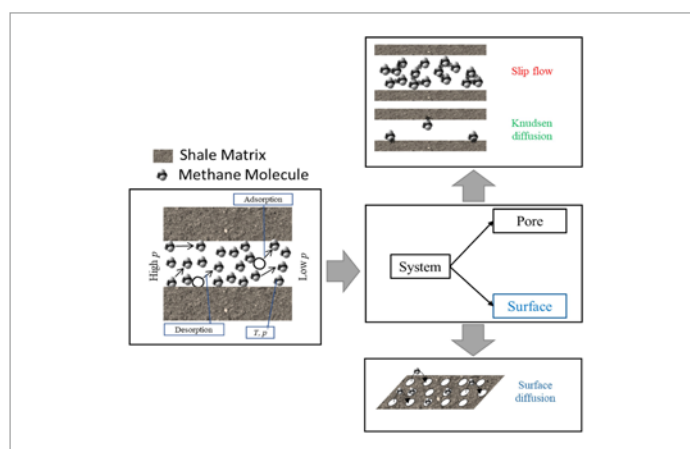


Fig. 1 - Conceptual depiction of the gas flow model analyzed in the PhD thesis. The overall gas migration is represented by the weighted sum of bulk flow and surface diffusion.

associated with unconventional energy production strategies and approaches for quantifying their environmental impacts under the presence of uncertainty are still needed. The PhD Thesis fills this gap upon developing and showcasing the use of a methodology for rigorous probabilistic risk assessment of potential groundwater contamination in relation to hydraulic fracturing operations. To exemplify the methodology, two contamination risk scenarios associated with hydraulic fracturing on sedimentary basins are formulated, whilst considering imperfect knowledge of (i) hydrodynamic parameters of system components such as fractures, source rock, and overburden permeability; (ii) operational conditions of the system such as water injection time; and (iii) geometrical features of the system components, such as location of preferential pathways and aperture of fractures. Detailed multicomponent flow numerical simulations and surrogate models

are employed to evaluate the probability density function of the quantities of interest for each risk scenario. Production allocation is then examined in the third part of the PhD Thesis. It is recalled that this is a technique for quantifying fractional contributions of individual oil sources (typically termed end-members) in a mixture thereof. Proper production allocation is critical in cases in which production facilities are shared to optimize production costs. Our work on production allocation is grounded on geochemical fingerprinting. The latter typically consists of two phases, i.e., (i) an experimentation phase (in which chromatograms of an oil mixture and their associated end-members are recovered) and (ii) a deconvolution phase (where algorithms are employed to treat the chromatogram data to assess the mass fraction of each end member in the mixture). The chromatogram associated with a given source of oil is often unique. Exploiting the difference

between chromatograms of differing sources is the foundation of production allocation based on geochemical fingerprinting. Traditional deconvolution techniques emerge from the application of so-called mixing models. These employ features of the end-member chromatograms to predict the same type of features of the mixture chromatogram. Peak heights mixing model considers the heights of chromatograms, whereas peak ratios mixing model employs the ratio of consecutive peaks. The latter has the relative advantage of being capable of dealing with chromatograms of poor quality under the reasonable assumption that ratios are less sensitive than peak heights to variations on the sample chemical composition caused by, e.g., improper storage of samples, or improper experimental conditions. Deconvolution can then be framed as an inverse modeling problem to quantify the relative contribution of each end member to the mixture. As a key result, a completely original deconvolution technique, termed PGM, is formulated. The approach relies on Maximum Likelihood estimation and employs the peak ratios mixing model. The original algorithm developed is also associated with a significantly reduced experimental cost in comparison with traditional deconvolution techniques also relying on Maximum Likelihood (Figure 2). The ensuing operational tool is now ready for routine industrial use.

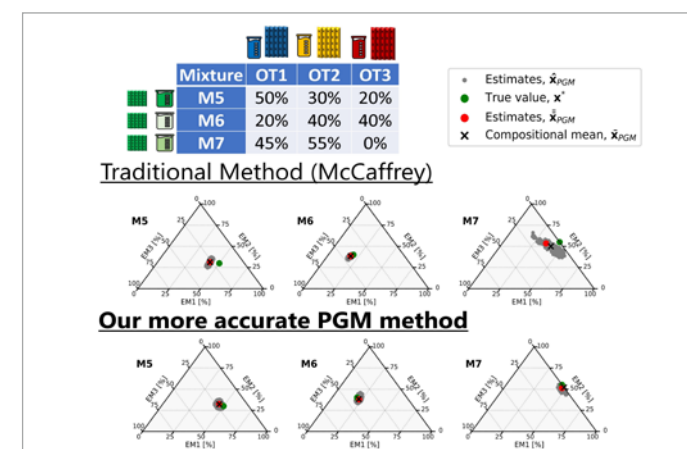


Fig. 2 - Ternary diagrams depicting the fractional contribution of end members to selected mixtures. More accurate and reliable predictions are obtained using our novel technique.

# HARNESSING HYDROGENOTROPHIC METHANOGENS

## ACTIVITY: EXPERIMENTAL AND MODELLING INSIGHTS ON H<sub>2</sub> TRANSFER

Anna Santus - Supervisor: Prof. Francesca Malpei

It is well known that climate change is a global emergency that requires immediate and substantial intervention in the energy system. The excessive dependence on limited fossil resources, coupled with the recent armed conflict in Eastern Europe, has exacerbated the energy crisis. In April 2022, the European Union (EU) issued the [REPowerEU plan](#), a plan aimed at encouraging member states to diversify their energy sources and consistently increase renewable resources. In this context, power-to-gas technologies are gaining interest due to their ability to connect renewable energy production with existing energy systems. Among these, excess renewable energy can be used for water electrolysis, producing green hydrogen (H<sub>2</sub>). This can be used directly as fuel or serve as a precursor for methane (CH<sub>4</sub>) production through carbon dioxide (CO<sub>2</sub>) reduction in the methanation process. Methanation from green H<sub>2</sub> can be catalysed chemically, in the presence of a catalyst or biologically, by harnessing the metabolism of hydrogenotrophic methanogenic microorganisms (*Archaea*), under milder operating conditions of temperature and pressure. Furthermore, the biological process can be more easily integrated with facilities where

anaerobic digesters already exist, providing a source of biogenic CO<sub>2</sub>. This doctoral thesis focuses on the detailed study of hydrogenotrophic methanogenesis in an *ex-situ* configuration. In this configuration, CO<sub>2</sub> is directly supplied to microorganisms with H<sub>2</sub> in a dedicated bioreactor. To date, the biological pathway has been demonstrated at the laboratory and demonstrative scale. The main technical issue highlighted in the literature is the ability to supply H<sub>2</sub> to microorganisms, emphasising the need to act on the gas-liquid mass transfer coefficient. Consequently, this thesis aims to thoroughly investigate the relationships within an *ex-situ* bioreactor, combining experimental and modelling activities. The primary focus is on the relationship between the H<sub>2</sub> transfer rate and the maximum H<sub>2</sub> consumption rate of hydrogenotrophic microorganisms. Literature has shown that measurements of activity (SHMA) of these microorganisms are strongly influenced by the system's ability to transfer the substrate, i.e., H<sub>2</sub>. SHMA values reported in the literature are frequently one order of magnitude lower than the maximum theoretical

uptake velocity ( $v_{max,CH_2}$ ) derived from the theoretical concepts of bioenergetics. Additionally, introducing a detailed biological model considering H<sub>2</sub> transfer and consumption by hydrogenotrophic methanogens could help understand and validate experimental results obtained from both batch and continuous *ex-situ* biomethanation activities. After exhaustively describing hydrogenotrophic microorganisms and the gas-liquid transfer theory, the thesis presents the experimental and modelling activities conducted during the doctoral research. Firstly, there is the introduction of the first implementation in OpenModelica of the mathematical model (based on ADM1) and the comparison of simulation results with two *ex-situ* experimental studies. A sensitivity analysis of the model has been conducted to understand which parameters significantly influence the model's variables, such as methane production and volumetric content in the final gas product. These parameters include the gas-liquid mass transfer coefficient ( $k_L a$ ) and the maximum uptake velocity of hydrogenotrophic methanogens ( $v_{max,CH_2}$ ). The

subsequent application of Linear Fractional Transformation (LFT) for parameter identification is proven to be a valuable tool, demonstrating good model accuracy. The value of  $k_L a$  for the thermophilic up flow reactor (UF) was 6 times higher ( $k_L a = 1532 \text{ d}^{-1}$ ) compared to that identified for the mesophilic continuous stirred tank reactor (CSTR) reactor ( $k_L a = 247 \text{ d}^{-1}$ ). Acknowledging the need for validation with additional experimental datasets is crucial to improve the model's robustness and expand its applicability. Then, the thesis focuses on the theoretical and experimental study of the maximum uptake velocity of hydrogenotrophic methanogens ( $v_{max,CH_2}$ ). This part firstly presents the calculation of the maximum consumption based on the concepts of the bioenergetic approach using the Thermodynamic Electron Equivalent Model (TEEM). Once the theoretical maximum consumption rate of hydrogenotrophic methanogens is identified, a method for experimental measurement of the activity of these microorganisms (SHMA) is studied. The absence of a standardized method initially led to a focus on the role of test operating conditions, such as mixing intensity, working liquid volume, and initial H<sub>2</sub> partial pressure in the headspace. The results of these tests demonstrated that SHMA values are significantly influenced ( $118 - 6'203 \text{ mL}_N \text{ CH}_4 \cdot \text{g VSS}^{-1} \cdot \text{d}^{-1}$ ) by operating conditions. In particular, maximum SHMA values were obtained for maximum mixing speeds, high hydrogen

partial pressures, and lower liquid volumes. These results confirm the dependence of the SHMA value on the transfer capacity established under different operating conditions. A maximum SHMA value of  $6'203 \pm 39.7 \text{ mL}_N \text{ CH}_4 \cdot \text{g VSS}^{-1} \cdot \text{d}^{-1}$  was achieved. This maximum SHMA value is one order of magnitude higher than mesophilic values reported in the literature and closer to the thermodynamic maximum estimated with bioenergetics concepts ( $9'806 \text{ mL}_N \text{ CH}_4 \cdot \text{g VSS}^{-1} \cdot \text{d}^{-1}$ ). These results were also confirmed by SHMA tests with dissolved H<sub>2</sub> measurements, where a limitation in H<sub>2</sub> supply is visible when  $k_L a$  is lower. The last part is focused on methods for the identification of the  $k_L a$  coefficient. Firstly, tests were conducted on a bioreactor ( $V_{liq} = 1 \text{ L}$ ) to determine the  $k_L a$  coefficient for hydrogen under standard conditions, i.e. in clean water ( $k_L a_{H_2} = 3'530 \pm 70.9 \text{ d}^{-1}$ ). Subsequently, the validation of this coefficient through modelling of *ex-situ* biomethanation experiments performed on the same bioreactor, identified a  $k_L a$  coefficient 20 times higher than that identified on clean water ( $k_L a_{H_2} = 65'568 \text{ d}^{-1}$ ). The much higher transfer rate of hydrogen identified could be explained by the enhancement factor theory following the model on  $E$  factor. To best of the author's knowledge, this factor has only been previously studied and reported in the context of oxygen fermentation. This result opens up new research avenues that could have significant technological

and operating impacts in terms of transfer devices and reactor configuration. However, systematic and more extended research is needed to elucidate and quantify this phenomenon. In conclusion, this PhD thesis makes a substantial contribution to advancing the comprehension of *ex-situ* biological CO<sub>2</sub> reduction to CH<sub>4</sub> with H<sub>2</sub>. The model is able to predict CH<sub>4</sub> v/v, meaning that it can be used as a tool for helping in design, control and optimisation of this biological process. Further investigations of the model include: i) studying intermittence of H<sub>2</sub> furniture, ii) inhibition pathways and inhibition constants identification, and iii) homoacetogenesis parameters sensitivity analysis and identification. These modelling developments should be implemented and validated with proper experimental analysis. Other experimental developments are related to the investigation of the microbial enhancement factor. All these future developments will help in speed up the scale up to industrial applications of the biomethanation process. The integrated approach of predictive modelling and experimental insights forms a robust framework, effectively addressing challenges and uncovering opportunities in the realm of renewable energy production.

## LAKES WATER QUALITY MAPS MONITORING AND DISSEMINATION: INSUBRIC LAKES CASE STUDY

Juan Fernando Toro Herrera - Supervisor: Prof. Daniela Carrion

The objective of this work is to assist public administrations in conserving water resources by monitoring various parameters of water quality to evaluate its overall status. The research focuses on addressing a specific area within geo-visualization, namely geographic visualization, and aims to develop efficient tools and web-based applications for the visualization, sharing, and automated processing of water quality parameters in inland water bodies.

The web-based applications, or Collaborative Data Sharing Platform and WebGIS, for sharing and monitoring the raster data have been implemented for a study case and are available on the Web. The Collaborative Data Sharing Platform enables the multitemporal visualisation of the water quality parameters maps for the study case. The platform benefits from open standards, free and open-source software, and open data, most notably to ensure interoperability and reduce the barriers to access it. On the other hand, the necessary tools and workflow for the semi-automated production of the water quality parameters maps are available inside a virtual environment for further development and applications to other study cases. A processing chain was implemented and integrated to generate maps of water quality parameters, in

the framework of SIMILE Interreg Italy-Switzerland project, which defined the algorithms to be used. This involved determining the most appropriate workflow and implementing a series of procedures to address issues encountered during map production. These identified issues, such as misaligned maps and the presence of anomalous values, had the potential to cause misinterpretation of parameter trends over time. Therefore, the processing chain integrated a co-registration

algorithm and statistical inference methods for addressing the issues. The primary goal of this research is to bridge the divide between scientific knowledge and society by effectively sharing research findings and enabling the use of web-based tools and containerised solutions for replication the work. By doing so, it aims to facilitate informed decision-making concerning different water quality phenomena.

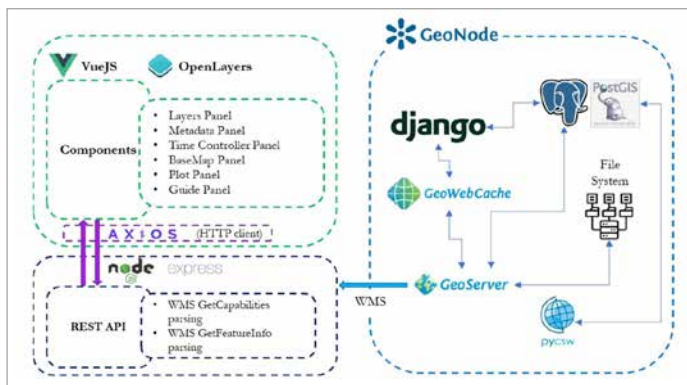


Fig. 1 - Collaborative data-sharing platform architecture. WebGIS (left-side). GeoNode (right-side).

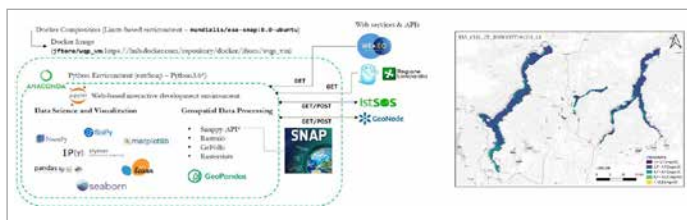


Fig. 2 - Virtual machine for the processing and sharing of WQP maps and statistics