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THE INFLUENCE OF VEGETATION DISTRIBUTION ON WETLAND EFFICIENCY

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Abstract

The increase of the construction of wetlands that there has been in recent years led the research to study all the processes involved in this kind of environment, with the aim of improving the design of these areas.

In particular, the goal of this research work is to investigate the influence that vegetation distribution may have on the wetland efficiency from a statistical point of view.

The tests were made using a 2D numerical model, and then the final results have been analyzed trying to find a relationship between the statistics of the vegetation and the efficiency of the wetland both in terms of concentration and mass.

La diffusione delle aree umide costruite verificatasi negli ultimi anni, ha portato la ricerca ad analizzare in profondita' i vari processi legati a questo tipo di ambiente, con l'obiettivo attraverso un' adeguata progettazione di aumentarne l'efficienza.

In particolare lo scopo di questa ricerca e' di capire in che modo i parametri riferiti alla distribuzione statistica della vegetazione, possano influenzare l'efficienza di queste zone.

Le simulazioni sono state fatte considerando un modello numerico bidimensionale, e i risultati sono stati analizzati cercando di trovare una relazione tra i parametri statistici e l' efficienza, sia in termini di concentrazione che in termini di massa.

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Chapter 1

Introduction

Wetlands represent a transition zone between terrestrial and aquatic environments where both hydraulic and biochemical processes take place all together. Wetlands are mainly applied for the purification of domestic wastewater treatment, but sometimes also for the purification of industrial or agricoltural wastewater, in fact in this kind of environments common pollutants can be transformed in to harmless substances and nutrients, thanks to the large amount of biological activity that is acting inside.

This thesis is going to deal with free water surface wetlands (FWS). The removal efficiency of free water surface wetlands is controlled by the time spent by contaminants into vegetated zones. For this reason the success or failure of a treatment wetland is contingent upon creating and maintaining correct water depths and flows. Hence results to be very important to know and understand the hydraulic factor that relates the flow rate and the vegetation density.

In this research work it has been tried to observe how the efficiency of a wetland is influenced by the statistics of the vegetation. Differently from the most common methods for designing wetlands in this case it was possible to take in to account the different flow paths that the water can have, related to the vegetation distribution. The work may be subdivided in six main parts:

- an introduction on humid areas features and on the processes that take place inside of them;

- a brief reviw of the most common theories used for wetland design;

- the definition of the hydrodinamic and solute transport models;

- the creation of a numerical matrix respresenting the density distribution in space of vegetation which will be used as input for the model, using HydroGen code;

- the resolution of the model by solving the partial defferential equations numerically, using Comsol Multiphysics;

- the analysis of the final results, trying to find a relationship between the statistical parameters of the vegetation and the efficency of the wetland.

Humid Areas

Wetland are defined as those areas that are inundated or saturated by surface or ground water at a frequency and duration sufficient to support, and that under normal circumstances do support, a prevalence of vegetation typically adapted for life in saturated soil conditions. Wetlands generally include swamps, marshes, bogs, and similar areas.

Natural wetlands have been used as convenient wastewater discharge sites for as long as sewage has been collected (at least 100 years in some locations). An example of old wetland site in North America include the Great Meadows natural wetland near the Concord River in Lexington, Massachusetts, which began receiving wastewater in 1912. Wetlands constructed for the purpose of treating water have a much shorter history. The worldwide spread of this technology originated from research conducted at the Max Planck Institute in West Germany, starting in 1952 [*Bastian and Hammer*, (1993)] and in the western hemisphere during the 1970s. Implementation of wetland technology has been accelerating around the world since 1985, primarily because treatment wetlands, while mechanically simple, are biologically complex systems capable of achieving high levels of treatment. Other benefits provided by wetlands include the possibility of water supply, a good water control, exploitation for mining, the use of plants they contain, the presence of animals in the wild, the presence of fish and invertebrates, control

of erosion and desertification, a great contribution to biodiversity, the possibility of use as an energy source, and finally for educational and recreational activities. Furthermore, treatment wetlands can be constructed using local materials and local labor, which is a major advantage in developing countries.

The artificial wetlands offer respect to natural ones a greater degree of control, allowing a precise evaluation of their effectiveness on the basis of the knowledge of the substrate nature, the types of plants and hydraulic paths. Constructed wetlands can provide other advantages such as: site selection, flexibility in the choice of size and geometry, and more importantly, an easier control of the flow and of the hydraulic retention time.

In these systems, the pollutants can be removed by a combination of chemical, physical and biological agents, including sedimentation, precipitation, adsorption, assimilation by plants and microbial activity [*Brix*, (1993)].

Figure 2.1. Free water surface wetlands.

2.1 Types of Treatment Wetlands

Modern treatment wetlands are man-made systems that have been designed to emphasize specific characteristics of wetland ecosystems for improving treatment capacity. There are three main types of treatment wetlands:

- Free water surface (FWS) wetlands, which contain areas of open water, floating vegetation, and emergent vegetation, and they are similar in appearance to natural marshes.

- Horizontal subsurface flow (HSSF) wetlands, where the wastewater flows through a gravel media planted with wetland vegetation. The water is kept below the surface of the bed, and it flows horizontally from the inlet to the outlet.

- Vertical flow (VF) wetlands, which distribute water across the surface of a sand or gravel bed planted with wetland vegetation. The water is treated as it percolates through the plant root zone. Biosolids dewatering wetlands can be thought of as a type of VF wetland system.

Each of these major categories employs variants of the layout, media, plants, and flow patterns.

2.1.1 FWS Wetlands

FWS systems consist in a series of tanks or channels where the water surface is exposed to the atmosphere, while the soil constantly submerged, acts as a support for the emergent plants. As the wastewater flows through the wetland, it is treated by the processes of sedimentation, filtration, oxidation, reduction, adsorption, and precipitation. Because FWS constructed wetlands closely mimic natural wetlands, it should be no surprise that they attract a wide variety of wildlife: insects, mollusks, fish, amphibians, reptiles, birds, and mammals (NADB

database, 1993; *Kadlec and Knight* (1996)).

Due to the hazard for human exposure to pathogens, FWS wetlands are rarely used for secondary treatment (U.S. EPA, 2000c), while they are commonly used for advanced treatment of effluent from secondary or tertiary treatment processes (e.g., lagoons, trickling filters, activated sludge systems.

FWS wetlands are suitable in all climates, including the far north. However, ice formation can hydraulically preclude winter operation, and the rates of some removal processes are lower for cold water temperatures, notably nitrogen conversion processes. When ice covers the open water, the transfer of oxygen from the atmosphere is reduced, decreasing oxygen dependent treatment processes. Other processes, such as TSS removal, are more effective under the ice than in summer conditions. It is generally more efficient to store water during winter and treat it during the warm part of the year.

FWS wetlands are the nearly exclusive choice for the treatment of urban, agricultural, and industrial stormwaters, because of their ability to deal with pulse flows and changing water levels. They are a frequent choice for treatment of mine waters, and for groundwater remediation and leachate treatment. FWS systems are usually capital cost-competitive with alternative technologies, and the operating costs are typically quite low. The components in a typical FWS wetland are shown in Figure 2.2[*Kadlec and Wallace* (2008)].

2.1.2 HSSF Wetlands

HSSF wetlands consist in gravel or soil beds planted with wetland vegetation. They are typically designed to treat primary effluent prior to either soil dispersal or surface water discharge.

The wastewater is intended to stay beneath the surface of the media and flows in and around the roots and rhizomes of the plants. These are usually anoxic
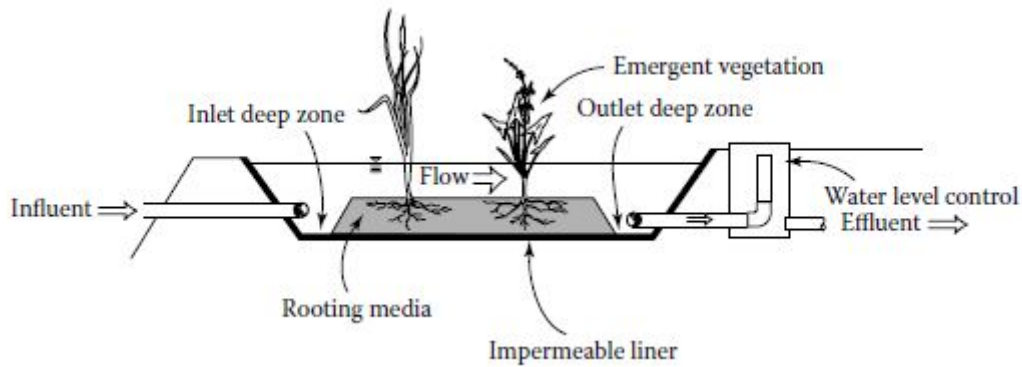
Figure 2.2. Basic elements of a FWS wetland.

environments with many aerobic areas around the plant roots. This presence of different redox conditions make it very elastic and adaptable for a large range of different types of wastewater. They are commonly used for secondary treatment, for single-family homes, for small cluster systems [*Kadlec and Wallace* (2008)], or for small communities [(*Cooper*, (1996)]. However, there are many other applications for particular wastewaters from industry. HSSF wetland systems are generally more expensive than FWS wetlands and they are utilized for smaller flow rates.

HSSF wetlands are typically comprised of inlet piping, a clay or synthetic liner, filter media, emergent vegetation, berms, and outlet piping with water level control. These systems are capable of operation under colder conditions than FWS systems, because of the ability to insulate the top. A key operational consideration is the propensity for clogging of the media.

HSSF wetlands do not provide the same opportunities for ancillary benefits that FWS systems do. Because the water is not exposed during the treatment process, the risk associated to human or wildlife exposure to pathogenic organisms is minimized. A schematic representation of a conventional HSSF wetland for warm climates is depicted in Figure 2.7.
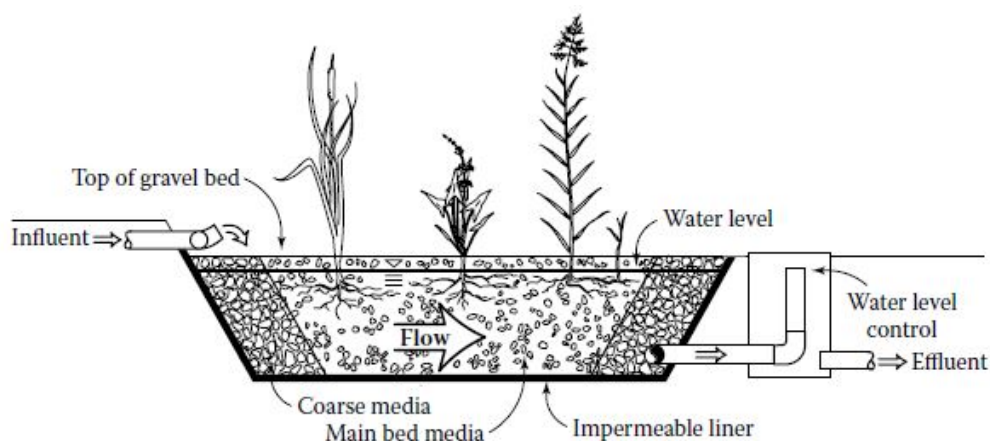
Figure 2.3. Basic elements of a HSSF wetland.

2.1.3   VF Wetlands

There are several variations of VF wetlands. The most common type used in Europe, employs surface flooding (pulse loading) of the bed in a single-pass configuration. Such systems are roughly analogous to the dosing scheme used in intermittent sand filters. Respect to HSSF wetlands which have a limited capacity to oxidize ammonia, because of limited oxygen transfer, VF wetlands were developed to provide higher levels of oxygen transfer, thus producing a nitrified effluent. For this reason VF wetlands are usually used in applications with ammonia content higher than municipal or domestic wastewater, such as: landfill leachates and food processing wastewaters, which can have levels of hundred milligrams per liter of ammonia.

These systems may be combined with HSSF or FWS wetlands to create nitrification-denitrification treatment trains. Another variation of VF wetlands relies upon exactly the opposite process: the use of overlying water to block oxygen transport, in order to create anaerobic conditions in the bottom bed sediments. A surface water pool on top of organics and limestone creates downflow into a zone with reducing conditions that fosters appropriate sulfur chemistry to immobilize metals [*Younger*, (2002)]. Also sludge from activated sludge plants may be dewatered

in VF systems [*Nielsen*, (2004)].

Biosolids dewatering wetlands consist of an enclosed basin with alternating filter layers which trap organic biosolids on the surface of the wetland bed. Biosolids are applied to the surface of the wetland bed, and water percolates vertically down through the wetland bed primarily through mechanisms of unsaturated flow.

Sludge dewatering system targets are water removal and consolidation, rather than the elimination of dissolved constituents. Sludge dewatering beds consist of an enclosed basin with a sand layer underlain by drainage pipes. The sand bed is planted with emergent wetland plants (typically Phragmites), and fed throughout the year in intervals with up to 20 cm of stabilized sewage sludge per loading [*Barjenbruch*, (2002)]. Solids content after dewatering is typically about 35-40 per cent [*DeMaeseneer*, (1997)]. Higher solids contents may be achieved, but this usually requires sacrificing the plants to drought stress [*Nielsen*, (1990)]. Freezing conditions enhance performance since ice crystals lyse the cell walls of the bacteria in the biosolids [*Reed*, (1995)].

Below a typical arrangement of a VF constructed wetland is reported (Figure 2.4)

2.2   Application fields

The application of Constructed Wetlands for the treatment of wastewater is nowadays a choice widespread in most of the world. In Italy this type of system is an ideal solution to meet the need to ensure a greater purification service, and to adapt existing systems in order to reach new objectives without involving a charge of investment and management levels. Constructed Wetlands, are mainly adopted for:

- Secondary treatment for small communities. For example, Green and Up-
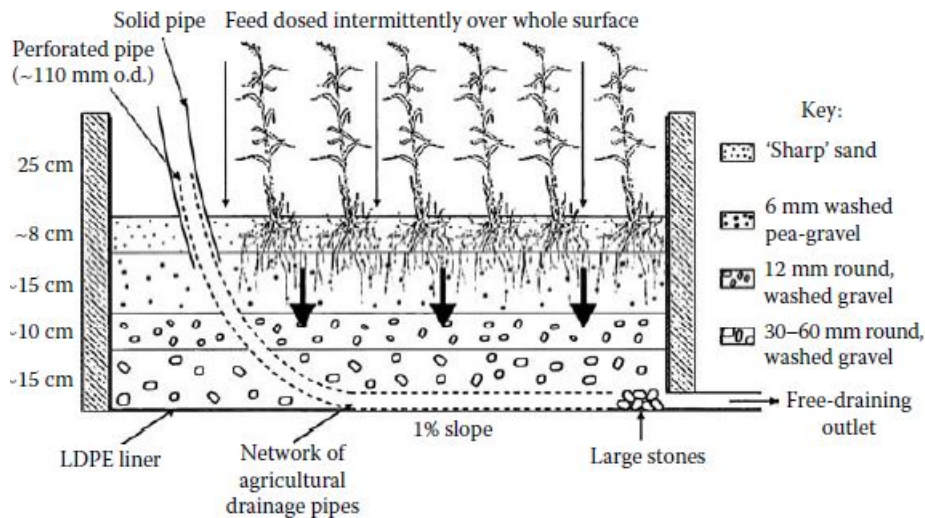
Figure 2.4. Basic elements of a VF wetland.

ton (1992) analyzed the costs for HSSF systems in the United Kingdom, and concluded that they were the technology of choice for villages of up to 2,000 population.

- Add-ons to aging or overloaded conventional secondary plants. The wetland acts as a buffer to complete the treatment when there are upsets or extreme flow events that create bypass and concentration excursions in the conventional plant outflow.

- Add-ons to lagoons. The solids trapping properties of wetlands can compensate for the export of algal debris from facultative ponds, and provide further nutrient removal.

- Tertiary and higher treatment of compliant secondary discharges. Changing regulatory requirements can create the need for advanced treatment, which may be provided by constructed wetlands.

Both the secondary and tertiary treatment systems, represent a good solutions, capable of having excellent yields (especially for parameters such as COD, BOD5, suspended solids and nitrogen), with environmental impact and energy con-

sumption significantly reduced compared to the other depurative systems.The tertiary treatments can be also applied to wastewater systems previously cleaned with chemical-physical and/or oxidation plants (activated sludge plants, biodisk plants, etc..), whose characteristics do not meet the limits imposed by law. In particular, they are mainly used for:

- breakingdown of nitrogen;

- reduction of organic substances that have slow times biodegradability and therefore require longer retention times;

- reduction of phosphorus;

- reduction of heavy metals;

- improving the microbiological and chemical quality of the effluent.

2.3   Pollutant reducing processes

The wetlands are very complex systems that separate and transform pollutants by physical, chemical and biological processes that can be performed simultaneously or sequentially during the stay of the water within the area. The processes, which together represent the purification capacity, are well known from a theoretical and quality point of view; however, their nature and their close interconnection has prevented, for some of them, of being able to acquire experimentally in situ evidence of knowledge.

The two main mechanisms which can be attributed to the self-purification capacity of a wet area are the separation of the solid phase from the liquid and the transformation of the substances present in the water. Here are reported the most important processes that determine the removal of the following class of pollutants in wetlands: suspended solids, nitrogen, phosphorus, organic matter, pathogens and heavy metals.

2.3.1   Suspended Solids

It is defined total suspended solids (TSS) those solids that are retained by a glass fiber filter (WHATHMAN GF / F). The amount of suspended solids that affects the inner cicle of solids (suspended and sediment) in wetlands is normally higher than the incoming load. Within a wetland in fact, the suspended solids are affected by both removal and production processes related to the death of invertebrates, the fragmentation of plant tissues, the production of phytoplankton and bacteria and the formation of unsolved compounds such as sulfides of iron.

The main processes for TSS removal are sedimentation and filtration. The process of sedimentation is a physical process controlled by some parameters such as the difference of density between the suspended matter and the water, the size and shape of the particles, the water viscosity, the turbulence and the type of the flow. Sedimentation may concern, however, even particles that reach the necessary conditions for them to fall trough aggregation mechanisms with other particles or substances (flocculation). In these cases, the presence of surface charges, or the spontaneity of certain reactions, allow to dissolved substances, or particles that are not sedimentable, to participate in the transformation processes which promote their aggregation and sedimentation by gravity.

The flocculation is favored by the relative movement of the particles which increase the probability of collision. Also the turbulence induced in a wet area by the presence of emergent vegetation, increases the probability of collision, even if the adhesion of these particles remains high dependent on the electrical surface properties that are themselves influenced by the quality of the surrounding water. In summary, the heavier particles, which in surface waters are kept in suspension by speed and turbulence greater than those present in wetlands, will settle near the emtrance points, while the sedimentation of smaller particles will depend on the residence time, on their specific chemical and physical character-

istics and on the water quality.

Filtration in the strict sense is not a very important process in wetlands. The density of the emergent parts of plants and the debris porosity in the superficial part of the bed are not enough to engage an effective filtration. However, the stems of the plants and the sediment-water interface are covered with a biofilm, composed of various types of organisms (bacteria, algae, fungi, protozoa) capable of effectively intercept the particles that pass through them. This biofilm can simply hold the particles that collide, or it can metabolize and dissolved these substances or colloidals, with production of biomass and soluble materials.

The efficiency of interception depends on the water flow, the density and size of the particles, the characteristics of the particles and the substrates of the biofilm. The lighter sediments can also be reported in suspension as consequence of a releasing from the bottom of gaseous substances, produced by photosynthesis and by the anaerobic decomposition of organic matter, which in their lift they transport solid particles in the water column, or as a result of strong winds inducing a wave motion capable of exerting a force on the bottom sufficient to bring the lighter sediments in suspension.

2.3.2 Nitrogen

In surface waters the most interesting forms of nitrogen are nitrate, nitrite, ammonia and organic nitrogen. All these forms, including gas nitrogen, are biochemically interconnected and they participate in the nitrogen cycle (Figure 2.5). The nitrogen as nitrate and to a lesser extent as ammonia, is an important nutrient for primary production. Its large presence in the waters, mostly due to the use of fertilizers and the oxidation of organic forms and ammonia contained in wastewaters, is one of the main causes of eutrophication of the waters.

The nitrogen can be removed both through chemical and biochemical reactions, that constitute together the nitrogen cycle, but also through physical separation.

In this second case, the same considerations made for suspended solids including processes such flocculation, sedimentation and filtration are true.
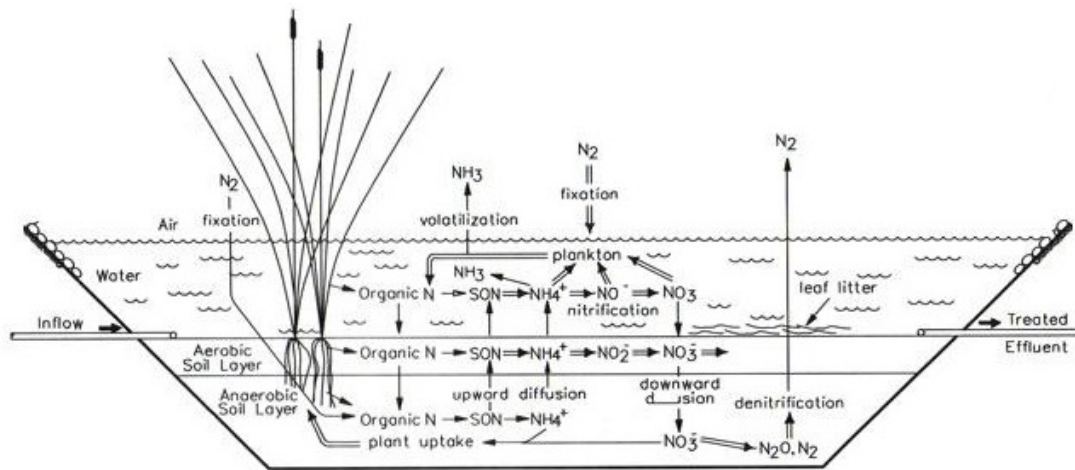
Figure 2.5. Nitrogen cicle in wetlands.

The bio-chemical transformations involving the nitrogen within the wetland are complex since this element in nature has an oxidation number varying from $-III(NH_3)$ a $+V(NO_3^-)$.

The vegetation is a temporary storage for nitrogen, in the short term: this function is performed by the process of assimilation which allows the use of inorganic nitrogen compounds for the synthesis of organic macromolecules that make up the plant biomass. The emerging macrophytes and, in part, the submerged ones assimilate the mineral nutrients in dissolved form through the roots located in the sediment, while phytoplankton and floating macrophytes assimilate the nutrients dissolved in the water column.

The organic matter resulting from the death of the organisms and from the settlement of suspended solids, is decomposed with the release of organic nitrogen, usually in a dissolved form (urea, amino acids, proteins). The mineralization is the process that transforms this element from an organic form to an inorganic one of ammonium ion (NH_4^+). This process strongly temperature dependent, can

take place both under anaerobic and aerobic conditions. The mineralized nitrogen in the soil can be taken up by plant roots, go back into the aqueous phase or it can be the subject of other biochemical transformations. In particular, the ammonium ion can participate in the ion exchange in the presence of clay if it reaches the sediment (by diffusion or decomposition of organic matter). Anyway this exchange capacity is a short-term potential because it is subjected to saturation. In an aerobic environment it is achieved the nitrification of NH_4^+. This process involves the transformation of ammonium ion (NH_4^+) into nitrate (NO_3^-). This transformation has two phases that take place thanks to two microbial species (Nitrosomonas and Nitrobacter), involving enzymes and specific cytochromes of the bacteria in question, and can be summed up by the following two chemical reactions:

$$2NH_4^+ + 3O_2 \rightarrow 2NO_2^- H_2O + 2 + 4H^+ + 142.2 cal \qquad (2.1)$$

$$2NO_2^- + O_2 \rightarrow 2NO_3^- + 37.6 cal \qquad (2.2)$$
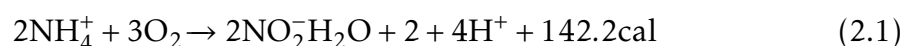
These are redox reactions whose velocity depends on the temperature, the redox potential and pH. Because the type of reagents required, these reactions take place only in the presence of oxygen and, therefore they take place in the aqueous phase by the microbial film attached on the vegetation, in the oxidized layer of the sediment in contact with water or oxidizing environment created by plants marsh around their roots and aerobic micro-climates created by bioturbation.

An intermediate product of nitrification is nitrite (NO_2^-) which is generally found in very low concentrations because its oxidation is much faster than production. The produced nitrate may follow different fates: in the soil it can be absorbed by plants through their roots, or, in presence of reducing conditions (anaerobic conditions), it can be denitrifiid by facultative anaerobic bacteria. They use the nitrate instead of oxygen as electron acceptor in the respiration process. The

stoichiometry of denitrification process can be represented in this way:

$$NO_3^- + H^+ + (CH) \rightarrow H_2O + \frac{1}{2}N_2 + CO_2 \qquad (2.3)$$
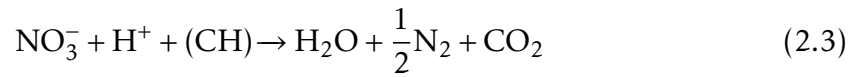
The denitrification brings to the production of molecular nitrogen in gaseous form which returns to the atmosphere passing through the sediment and eventually through the plant tissues. A peculiar aspect of this process is the transfer of nitrogen from the aqueous matrix to the atmosphere that represents an appreciated type of removal in water purification processes.

As it can be seen from the stoichiometry, the denitrification requires an oxidized form of nitrogen and an anaerobic environment; two conditions conflicting to each other. Hence in wetlands, denitrification becomes a significant process, thanks to the presence of aerobic micro-zones, which are necessary for the synthesis of nitrate, surrounded by anaerobic environments, required for denitrification.

The presence of these two types of conditions (aerobic and anaerobic) is found around the roots (rhizosphere) of typycal wetland plants, which live rooted in anaerobic sediment and that transfer oxygen from the air to the sediment through the root systems. Similar conditions are also in the sediment-water or more generally in biofilm-water surface. Many processes of assimilation and denitrification in fact occur in the water column by phytoplankton communities and bacteria in the biofilm.

The denitrification reaction requires a source of organic carbon, which in some cases can be a limiting factor. While the limitation by nitrate almost never occurs, due to the type of water which has to be treated, that is generally rich in this compound, the limitation by carbon in a wetland can be expected through the determination of appropriate parameters, such as the ratio C/N.

Other processes involving nitrogen within the wetland, are the volatilization of

ammonia and the fixation of atmospheric nitrogen. In the first transformation that takes place in the presence of high PH and high temperatures the ammonia (NH_3) goes into the gas phase and it is released in the atmosphere. It may become relevant during the warm months when the photosynthetic production can induce high PH (around 8.5). Of opposite sign is instead the fixation of atmospheric nitrogen that allows some organisms to use it as a nutrient for their growth.

2.3.3 Phosphorus

Phosphorus is present in surface water as soluble inorganic phosphorus, mainly as orthophosphate, and as organic phosphorus, both in dissolved and particulated form. The orthophosphate or soluble reactive phosphorus is biologically active, and it often reppresents, for the primary producers a nutritional limiting factor. For this reason it is in the composition of fertilizers and constitutes. With nitrogen salts, itis one of the responsible substances for the eutrophication.

The phosphorus cycle (Figure 2.6) does not have a gaseous phase and this leads to a gradual loss of this element in the sediments of water bodies. This happens also within the humid areas where the subtraction of phosphorus is related to its immobilization in the sediments, that with time are buried and then subtracted to the biological activity of recycling of the elements.

The removal of orthophosphate is promoted both by biological processes, such as assimilation by plants, and by chemical and physico-chemical processes (adsorption-desorption, precipitation, complexation) that favor the removal from the water column through sedimentation. The assimilation of organic phosphorus by the plants through the root system plays a lesser role than for the nitrogen in fact it is possible to consider that every 7 grams of nitrogen it is assimilated about 1 gram of phosphorus.

The link between the soluble form and the solid particles is established through
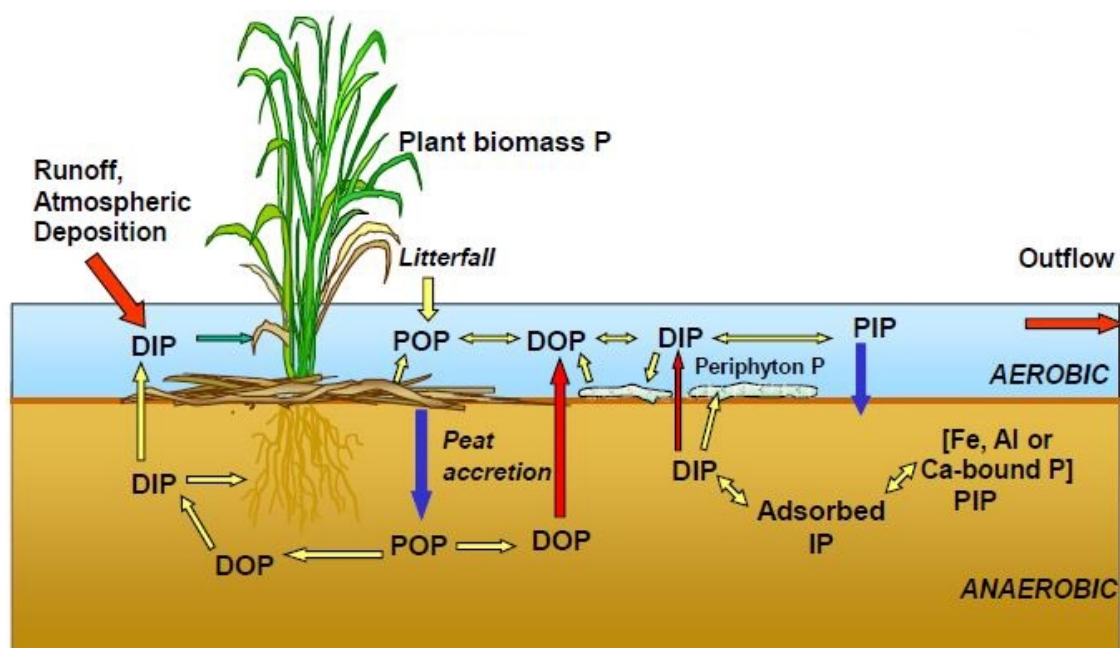
Figure 2.6. Phosforus cicle in wetlands.

the adsorption process by which it has the passage of a substance from the aqueous phase, to the surface of a solid phase. In this case the process takes place very quickly, so it may think that the phosphorus enters to the wetlands mainly as adsorbed to the suspended matter.

The exchange of soluble phosphates by diffusion and adsorption/desorption, between the pore water of the sediment and the water column is the most important path for this chemical species in the wetlands. In the pore water phosphorus may form precipitated particles by reacting with elements such as iron, calcium and aluminum, or it can be adsorbed by clay particles and organic fractions present in the sediment. However all these processes are reversible and they are controlled by environmental conditions such as pH and redox potential. For example in anoxic conditions, the decrease of the redox potential favors the reduction of ferric ion to ferrous ion ($Fe_3^+ + e^- \rightarrow Fe_2^+$), with the production of soluble compounds and with the consequent release of phosphate. In anoxic conditions you may also have release of phosphate boundded to iron and aluminum by hydrolysis.

Despite the reversibility of the processes discussed above, in the long term you will usually get a subtraction of phosphate thanks to the gradual burial of the sediment. In fact, the Phosphorus bounded to the sediments will be physically isolated with a reduced mobility, over time. The organic phosphates are assimilated by plants only after being mineralized by the action of microbial flora. The bacterial flora contributes to immobilize part of the dissolved organic phosphorus, or to increase the pool of dissolved inorganic phosphorus through hydrolysis processes and through anaerobic decomposition or mineralization, depending on which species are involved. Actually, the residence mechanisms of dissolved phosphorus in wetlands are not very efficient; appears, however, much more significant results to be the removal of phosphorus associated with suspended solid particles subjected to sedimentation.

2.3.4 Organic substances

The composition of the organic matter in surface water is complex, because it consists of many chemical compaunds present in low concentrations. For this reason it has to be evaluated by using parameters that take into account all the organic compounds present in the sample, such as: BOD (oxygen demand for biological oxidation), COD (oxygen requirement for the chemical oxidation) and TOC (total organic carbon).

The organic substance can be present both in soluble and particulate form. In particulate form it is subjected to flocculation and then to sedimentation, interception, absorption by the biofilm that covers the plants and the water-sediment interface, and mineralization by the microbial flora. Instead, dissolved organic matter may be assimilated and decomposed by microorganisms in the biofilm and in the sediment. Then it can be associated with the solid phase present in the water column and sediment through adsorption and absorption processes, that control the distribution between the solid phase and aqueous phase as function

of the features of different types of molecules (eg. lipophilicity, size and molecular weights). Some organic substances, characterized by high values of Henry constant, can also move from the aqueous phase to the air through the volatilization process. In a natural environment, the removal of biodegradable organic matter, takes place through subsequential biochemical transformations, made by a set of specialized organisms, which takes from this activity the energy and the substances needed to support themselves.

The demolition of the organic substance, allows the exploitation of the energy released during the redox reactions, that involve the transfer of electrons from organic compounds to substances, that act as electron acceptors. The environment can markedly influence the type of biochemical transformation. For example, the availability of oxygen as a final electron acceptor, allows a series of reactions that constitute the aerobic respiration. With no oxygen, that is a frequent condition in the sediments, other organic or inorganic substances such as nitrates, sulfates and carbonates are used as electron acceptors (anaerobic respiration). Hence, the environmental conditions, in terms of dissolved oxygen content, estabilish which type of degradative metabolism is feasible, and consequently the final products of the degradation process: carbon dioxide and water for aerobic respiration and, for example, oxides of nitrogen, nitrogen gas , sulfides, thiosulfates, hydrogen, methane, for anaerobic respiration. Aerobic respiration in terms of energy is more efficient than anaerobic.

The decomposition of organic matter can change in an important way the water quality of the wetland: aerobic respiration consumes dissolved oxygen while the anaerobic one produces unwanted substances. However, this aspect is usually not relevant in wetlands for the treatment of surface waters, because the modest load of organic substances to which they are subjected; while it can assume considerable importance in wetlands for the treatment of some specific wastewater that is rich of organic matter.

2.3.5 Pathogenic organisms

The pathogenic micro-organisms present in the water are viruses, bacteria, fungi, protozoa and helminths. Directly measurements are very expensive and usually it is entrusted to the quantification of more general indicators such as faecal coliforms, faecal streptococci and other classes of bacteria, that indicate their presence. However, that fecal coliform as well as some pathogenic microorganisms are also produced by the wetland fauna.Then the wetland is characterized by a baseline value.

The pathogenic microorganisms enter into the wetlands associated with suspended solids or as suspended colonies. If they are associated with suspended solids they will be subjected to the processes already seen for these compounds. Once they sedimented, the pathogenic orgnisms, adapted to live in warm-blooded organisms, are in a hostile environment. They require high temperatures and substrates rich in organic matter to live and generally they do not survive the competition with the community of environmental microorganisms. They may also be destroyed by ultraviolet irradiation if adequately exposed to sunlight. In any case the removal of pathogenic organisms, is related to the removal of suspended solids and factors such as the residence time.

2.3.6 Metals

The metals may enter into the wetlands in dissolved form or as insoluble compounds, associated to suspended solids. In the latter case, they undergo the processes of flocculation/sedimentation, filtration and interception. Instead the metals in dissolved form, may be taken from the aqueous phase for beeing associated with the solid phase, by processes of cation exchange and chelation with sediments or suspended solids; they can form bonds with the humic fraction of the sediment, they may precipitate as insoluble salts of sulfides, carbonates, hydroxides and they can be assimilated by plants, algae and bacteria. Depending from

the pH and the redox potential, insoluble compounds can be solubilized and return to the water column. However, the main fate of metals is to form compounds with the sulphides present in the anoxic sediment, forming compounds that will be buried with the sediment.

Resuspension and oxygenation processes of the sediments can reverse this path causing the solubilization of metals, which no longer bounded to the solid fraction, they return available in the aqueous phase. The assimilation of organic metals varies depending on the type of metal and the type of organism.

Today, there are no sufficient knowledge to estimates the removal of metals, however, the anoxic environment of the wetland sediments is an important factor for the immobilization and the burial of the metals deposited by suspended solids sedimentation.

2.4   Vegetation

The plants generally used in the constructed wetland systems are herbaceous typical of humid environments, and they can be divided into two main groups: the helophytes (or rooted emerging macrophytes) and hydrophytes.

The first group are plants that live on soils partially or completely saturated by water, up to a partial submersion of the stem, while leaves and flowers emerge from the water.

The second group have a vegetative body completely submerged or floating on the water surface, and they are considered aquatic plants in the strict sense.

Therefore the development of different plants take into account the water depth as the main environmental factor, in addition to other factors such as the characteristics of the soil, temperature, water quality, the competitive relationships between the different species. The main roles of vegetation in a wetland are:

- roots and rhizomes provide oxygen to the sediments;

- the submerged parts of the plants act as support for the biofilm that facilitates the nutrient transformations, increases the organic flocculation, filters the pollutants and promotes the sedimentation;

- the emerging parts of the plants provide protection from wind and sunlight resulting in a reduced temperature and a decreasing of algal growth;

- the presence of aquatic plants increase the head losses, creating complex paths in the flow, favoring the residence times and processes to reduce pollutants;

- the presence of vegetation increases biodiversity and provides a variety of habitats for macro-and micro-fauna;

Then, the reed would be planted in an appropriate manner to maximize the treatment efficiency of the wetland, to increase its value as natural habitat and its aesthetic and recreational value.

Figure 2.7. Examples of suitable plants for wetlands: helophytes - hydrophytes

2.4.1 Wetland Morphology

The morphology of a wetland is one of the most important design factors which determining the possibility of life and the development of macrophytes.

The wetland should have a low depth, and a ground sufficiently soft and exposed to the sun, in order to maximize the plant growth. Many plants adapted to wet areas grow faster in soils with sandy and silty texture, with a high organic content. Soils with excessive clay or rock material may retard plant growth up to mortality. Excessively acidic or basic conditions may limit the availability of nutrients required for growth. In some cases, the nutrients necessary for the plant growth may not be available in the original soil, in these case it will be necessary to use organic fertilizers.

2.4.2 Biodiversification

Usually the polycultures are preferable to monocultures, in fact in the second case, there is a greater probability of: invasion of weeds, destruction by pests, plant diseases. In addition, several plant species favor different types of habitat, providing different food sources and consequently increasing the biodiversity (both for aquatic species and birds)

. The alternation of vegetated and no vegetated areas with the length of the coastline are factors directly related to the biodiversity.These are the reasons because it should be integrated spots of different plant species within the wetland.

The vegetation of a wetland provides a source of food for fishes, favorable habitat, where the shadow provides to control the temperature. However the presence of vegetation, can be harmful to fishes life if too thick: channels without vegetation, and water mirrors are necessary in fact for their displacement.

The high temperatures are a limiting factor for many aquatic organisms: the temperature can be controlled by providing shaded areas above vegetation, deep pools of water and areas with sustained flow. These areas of deep water, and

channels without vegetation will obviously follow meandered paths in order to prevent short circuits and hydraulic dead zones.

2.4.3 Density of vegetation and hydraulich considerations

The stem density of wetland plants is a very important factor. In fact the density of the vegetation must not be such as to inhibit the circulation of the water, but high enough to be effective in the purification processes and able to block the organic material transported by the current.

Depending on the plant type and on the location, the stem density can vary a lot. For instance, Nepf et al. (1997) used a range of stem (cylinders) densities between 200 and 2,000 per m^2 in constructed flume experiments, to represent Juncus roemerianus. High density vegetative in a wet area decreases the velocity of the water, forces the water to follow a longer path and holds it in the wet area for a longer time.

In general, densely vegetated areas are most effective in treating the pollutants compared to sparsely vegetated. The aspect ratio of the macrophyte zone will vary between 4:1 (length: width) 10:1. Ratios lower than 4:1 phenomena may cause a short circuit. Extensive vegetated areas provide a frictional resistance to the flow facilitating the processes of sedimentation. More extensive is the vegetated area, the higher is the potential ability to facilitate sedimentation. Vegetation with a high density, decreases the probability of re-suspension of sediments by the action of wind and wave. Hence into vegetated areas the plants should be planted in the perpendicular direction respect to the flow in order to reduce the risk of preferential pathways.

2.4.4 Stabilization of the coastline

The emergent vegetation, which persists for the entire year, will generally be able to provide a valuable contribution to the stability of the coastline, offering a resistance to the wave motion and holding the soil with its roots. The trees

planted along the banks, however, can in time lead to the collapses: the weight of the tree may eliminate the advantage given by the root system. The trees, and vegetation in general can be used as natural shielding to the wind in cases where the fetch is too long.

2.4.5 Primary production

The wetlands are often considered as one of the most productive biological systems for their ability to export large amounts of organic material. Primary productivity is higher in wet areas with moving water with laminar flow; instead high flow velocity discourage plant growth.

Primary productivity is highest in waters with a pH between 6 and 8.5; surface waters generally fall into this range of pH. Net production in natural wetlands not subject to nutrient enrichment by humans is between $50 g/m^2 year$ (Arctic tundra) and $3500 g/m^2 year$ (United States). In temperate climate, most of the marshes with moving water have a net production ranging from 600 to $3000 g/m^2 year$ [*Kadlec and Knight* (1996)].

2.4.6 Organic carbon sources for denitrification

When the plants inside a wetland mature and die, they form organic detritus. This represents a carbon source that is used as a substrate by microorganisms whose activities influence many of the water purification processes. The typical organic detritus of a mature wetland takes from 1 to 5 years to develop [*Kadlec and Knight* (1996)].

2.4.7 Water depth and vegetation

A wetland can be managed encouraging, discouraging or maintaining the presence of certain species of plants. The management of the hydraulic level combined with a design that has provided areas with different depths can be used to moderate or encourage colonization and for selecting specific plant communities.

A high hydraulic head can be used to eliminate plants in areas where they are not desired [Gradilone et al., 1997]. In table 2.8 there is a list of the most common plants suitable for different depths.

Tab. 3.9 Profondità tipiche di alcune piante adatte ad un'area umida		
Tipologia vegetale	**Nome della specie**	**Profondità tipiche (m)**
Emergenti	Typha spp.	da 0.1 a 1
	Phragmites spp.	da 0.1 a 1
	Scirpus spp.	da 0.1 a 1
	Juncus spp.	da 0.1 a 0.3
	Carex spp.	da 0.1 a 0.3
Sommerse	Potamogeton spp.	> 0.5
	Vallisneria spp.	> 0.5
	Ruppia spp.	> 0.5
	Nuphar spp.	> 0.5
	Elodea spp.	> 0.5
Galleggianti	Lemna spp.	suolo inondato
	Eichornia crassipes	suolo inondato
	Hydrocitlye umbellata	suolo inondato
	Azolla spp.	suolo inondato
	Wolffia spp.	suolo inondato

Figure 2.8. Suitable plants for common wetland depths [*Linee guida*, (2005)].

2.4.8 Vegetation types

The choice of the plant species in a wetland should consider: the water quality, the water depths of the project and in extreme conditions, climate, latitude, and the aims of the wetland. Nowadays, there is no experimental evidence showing that the purification performance are different between different species of rooted emerging macrophytes commonly used [*Kadlec and Knight* (1996)].
General criteria considered for chosing are: growth potential, resistance, the cost of planting and maintenance costs. Plant species that maintain their structure during the whole year allow a better purification performance than the species

that are die at cold temperatures. For these reasons, the emerging species characterized by high content of lignin, and that are able to adapt to variable water heights, are the most used in humid areas. The marsh plant species that most successfully meet these criteria include Phragmites, Typha and Scirpus [*Kadlec and Knight* (1996)].

2.4.9 Planting

The phase of planting is crucial for the successful realization of a wetland. Rarely it is possible to be confident on a natural colonization of the vegetation; in fact this process requires a longer time compared to the planting, with also the risk to obtain a vegetation that is not uniformly distributed.

The planting of the wetland should be done as soon as possible in the sequence of construction procedures. Because, often, it happens that during the initial stage of the wetland life, when the vegetation is not yet present, water quality is less than expected, because of algal growth, the re-suspension of sediments and animal activity in areas of low water designed to be vegetated. If the wet area has to be planted, the cost and availability of plant species should be verified during the first design stages. The possibility to achieve a nursery on the site nursery for transplantation should be decided in advance. In fact it is preferable plants of 1 or 2 years [*Kadlec and Knight* (1996)], having these sufficient energy reserves to survive to the transplant operations. Consequently, the creation of a nursery must be completed before the constructive operations. The success of planting will depend on the skill of the nurseryman, the type and quality of the plants, from the soil matrix and the period in which the planting is done.

The preparation of a suitable substrate will be based on horticultural principles, which take into account, the tolerability of the substrate to the plant growth, the ability of the roots to slip in the soil, the presence of nutrients. Usually the bottom of the humid after the excavation phase, it will be too compacted to allow

the growth of the plant roots and it could also be poor in nutrients. Therefore it is necessary to provide suitable substrates to the planting.

The minimum thickness of the substrate should be 25 cm and typically it is used a substrate coming from the construction of the wetland: the substrate material removed from the soil surface must be preserved and protected from erosion and then subsequently reused in the wet area after the excavations are completed. Substrates imported from outside of the construction site must be tested with regard to their ability to support plant growth, the presence of contaminants and their ability to retain nutrients. In any case it must be avoided the use of substrate containing weed seeds. Once positioned the substrate must be leveled without being compacted.

The fastest mode of planting is on damp or dry soil, that should be irrigated. If the planting phase will last for several days or weeks, it is necessary to provide a frequent irrigation.

2.4.10 The hydraulic residence time

Of great importance in the process monitoring and analysis of a wetland are the nominal hydraulic residence time and the hydraulic residence time distribution (RTD). The nominal residence time is not necessarily indicative of the real residence time, in fact its calculation is based on the assumption that the entire volume of water of the wet area is affected by the actual flow. This may not be true, and in general it never is, with the result that measured residence times are lower than the nominal value.

The RTD represents the time that the various water particles spend within the system and therefore it is the distribution of the contact time for the system. Then RTD is the probability density function for the residence time in the wetland. The RTD function can be determined by injecting an impulse of inert tracer (for example, lithium chloride) into the incoming wet area and then measuring

the concentrations of tracer in the outflow as function of time.

2.4.11   Water level and flow control

The control of water level and flow are often the only variables on which it can work to significantly affect the pollutant removal in a wet area. The water level influences: the hydraulic residence time, the speed of the water, the flooded areas, the diffusion of atmospheric oxygen, the coverage of the plants, the water temperature, the scattering of sunlight and the sedimentation processes.

The discharge influences the hydraulic loads, the loads of pollutants, the residence time, the water velocity. These variables in turn influence the water quality and the ecosystem health.

During the summer when the water temperatures are high, the potential saturation of oxygen is lower and plant productivity is higher, the water level should be lowered to allow better diffusion of oxygen to the sediments, the roots of plants and microbial communities that make purification. On the other hand a lower water head facilitates the further increase of the temperature and the diffusion of light that may cause an increase in algal productivity.

During periods when the water freezes, levels must be reduced by lowering the control structure in output, so that the water flows freely under an air gap below the cover of ice and snow. Water birds use the islands for nesting: at the beginning of the nesting period the water levels must be kept high, so that the birds are forced to build their nests in higher positions. This will allow for the possibility of future fluctuations in levels even during the nesting period, without the fear to flood the nests. Different hydraulic levels generally create a greater biodiversity . Drastic fluctuations in water level can cause serious damage and erosion should be avoided. The speed of fluctuations in the level must be sufficiently slow to allow the migration of benthic fauna: a change in the level of $30cm/day$ did not appear to affect benthic communities [$Smith$, (1981)], while fluctuations larger

than $90cm/day$ will ensure negative effects [*Fisher and Lavoy*, (1972)]. Sediment released into the marsh due to erosion can smother the roots of plants, especially trees. Even a soil with a high concentration of clay can help to dramatically reduce the diffusion of oxygen into the root zone.

Chapter 3

Common design model for wetlands

This chapter presents a review of the most common theories followed for designing free surface constructed wetlands (FWS). These methods are generally based on two theories: Pollutant Removal Theory and Hydraulic Design Theory. As it will be possible to observe, they take in to account only the density and not the other statistics of the vegetation distribution. In the last part of this thesis a comparison between this semplifyed approach and the approach that consider the spatial distributions of the vegetation will be made.

3.1 Pollutant Removal Theory

Before starting with this model, it is necessary to make a couple of assumptions:

- The water temperature can be assumed approximately equal to the mean ambient temperature. This is a reasonable assumption for relatively warm climates [*Kadlec and Knight* (1996)];

- The removal rates for the pollutants in FWS constructed wetland systems are typically based on first-order kinetics and on the assumptions of plug flow, and are based on the models proposed by the USEPA (1988) and *Reed et al.* (1995), which have been used in the design of most constructed wetland systems in the U.S. and Europe [*Tsihrintzis and Madiedo* (2000)];

Pollutant removal rates in FWS constructed wetlands can be estimated for the most common pollutant treated in wetlands by one of the following general equations[*Kadlec and Knight* (1996)]

$$\frac{C_e}{C_i} = e^{-K_T t} \tag{3.1}$$

$$\frac{C_e}{C_i} = e^{\frac{-K_1}{h_l}} \tag{3.2}$$

In these two general equations: C_e is the pollutant effluent concentration$[M/L^3;$

Pollutant	Equation used	Rate constant		Rate constant units
BOD	(1)*	$K_T = 0.678(1.06)^{T-20}$		$[d^{-1}]$
Fecal coliforms	(2)**	$K_1 = 0.3$		$[m\ d^{-1}]$
Nitrogen				
Nitrification	(1)*	$K_T = 0.0389T$	$0 < T < 1°C$	$[d^{-1}]$
		$K_T = 0.1367(1.15)^{T-10}$	$1 < T < 10°\ C$	$[d^{-1}]$
		$K_T = 0.2187(1.048)^{T-20}$	$T > 10\ °C$	$[d^{-1}]$
Denitrification	(1)*	$K_T = 0.023T$	$0 < T < 1°C$	$[d^{-1}]$
		$K_T = 1.15^{(T-20)}$	$T > 1\ °C$	$[d^{-1}]$
Phosphorus	(2)**	$K_1 = 0.0273$		$[m\ d^{-1}]$

Figure 3.1. Rate constants for most common pollutant treated in FWS constructed wetlands. [*Kadlec and Knight* (1996)]

C_i is the pollutant influent concentration$[M/L^3]$; K_T is a reaction rate parameter $[1/T]$ which depends on the water temperature T and on the kind of pollutant it is considering$[C°]$, and the pollutant of interest (3.1); K_l is a reaction rate constant $[L/T]$ dependent only on the pollutant of interest (3.1); h_l is the hydraulic loading rate$[L/T]$ and $t\ [T]$ is the hydraulic residence time (HRT) inside the wetland. The last two parameters are defined by the following equations:

$$h_l = \frac{Q}{A} \tag{3.3}$$

$$t = \frac{V}{Q} = \frac{Ay\phi}{Q} = \frac{y\phi}{h_l} \qquad (3.4)$$

where Q is the design flow rate $[L^3/T]$, assumed constant; A is the mean surface area of the system $[L^2]$; V is the system volume$[L^3]$; y is the flow depth $[L]$; ϕ is the fractional porosity, which expresses the space available for water to flow through the vegetation in the FWS constructed wetland system [*Reed et al.* (1995)]. The estimation of pollutant removal in FWS constructed wetlands results to be very easy, assuming that the water temperature T can be taken equal to the ambient temperature T_a [*Kadlec and Knight* (1996)], and thus t can be computed directly from Equation 3.1 or 3.2, depending on which pollutant it is considered, setting $T = T_a$ and using the appropriate kinetic rate constant from 3.1.

3.2 Hydraulic Design Theory

Kadlec (1990) proposed the following general equation for the hydraulic design of FWS constructed wetland systems:

$$Q = aWy^b S^c \qquad (3.5)$$

where Q is the flow rate $[L^3/T]$; W is the wetland width $[L]$; a, b and c are coefficients assuming the following values: $a = 107d^1 m^{-1}$ for dense vegetation, $a = 5107d^1 m^{-1}$ for sparse vegetation, b = 3.0 and c = 1.0; y is the depth of flow $[L]$, which usually ranges from 0.1 to 0.6m [*Reed et al.* (1995)]; and s is the water surface slope $[L/L]$, which can be estimated by the following equation:

$$S = \frac{\Delta_y}{L} \qquad (3.6)$$

where Δ_y is the fraction of the depth serving as head differential [*Reed et al.* (1995)]; and L is the wetland length $[L]$. Equation 3.5, with the values of the

coefficients a, b and c mentioned above, seems to describe accurate flow through wetland vegetation [*Kadlec* (1990)]. Alternatively, Manning's equation can also be used, if a, b and c in 3.5 are set equal to $1/n, 5/3$ and $1/2$, respectively, with n as the Manning's roughness coefficient.

Many experiments has shown that the Manning's coefficient values for wetland vegetation are significantly higher than those for turbulent open channel flows controlled by skin friction. Indeed, flow resistance in wetland vegetation is highly dependent on the type, height and density of vegetation, the diameter and flexibility of the vegetation's stem, the depth of flow, the depth of litter layer, etc.[*Kadlec and Knight* (1996)]. If Manning equation is to be used, then the Manning's roughness coefficient n can be estimated with one of the following three methods:

- Using the data, procedure and design graphs provided by *Tsihrintzis and Madiedo* (2000), where n is presented as a function of VR_H (product of mean velocity and hydraulic radius), vegetation density and other factors.

- Using a logarithmic diagram developed by *Kadlec and Knight* (1996), based on information from existing wetlands, which allows for the preliminary estimation of Manning's roughness coefficient n as a function of flow depth. To simplify the use of this diagram,*Tsihrintzis and Madiedo* (2000) have developed two regression lines of the following general equation:

$$n = \beta_1 y^{\beta_2} \tag{3.7}$$

where: $\beta_1 = 0.1564$ for sparse vegetation and 1.09 for dense vegetation; and $\beta_2 = 1.356$ for sparse vegetation and 1.436 for dense vegetation.

- Using the general 3.7, but with the following values for coefficients β_1 and β_2, proposed by *Reed et al.* (1995): $\beta_2 = 0.5$; $\beta_1 = 0.4m^{\frac{1}{6}}s$ for sparse and low-standing vegetation with flow depth $y > 0.4m$; $\beta_1 = 1.6m^{\frac{1}{6}}s$ for moderately dense vegetation with flow depth y in the range 0.3 to 0.4m; and

$\beta_1 = 6.4 m^{\frac{1}{6}} s$ for very dense vegetation with litter layer and with $y < 0.3m$. In most FWS constructed wetlands, β_1 ranges from $1 m^{\frac{1}{6}} s$ (sparse vegetation) to $4 m^{\frac{1}{6}} s$ (dense vegetation).

It is noticed that in most FWS constructed wetland systems there is water surface control at the outlet. Thus, the depth may not be normal close to the outlet. However, it will tend to normal depth further upstream, particularly if the wetland is designed with a large length to width ratio, something generally recommended. In any case, the downstream control depth can be set close to normal depth. As suggested by *Kadlec and Knight* (1996) , the aspect ratio $L : W$ should be greater than 2:1 to ensure plug flow conditions.

However, very high ratios may result in overflow problems due to resistance increase as a result of the gradual accumulation of vegetation litter. Commonly used aspect ratios are between 2:1 and 5:1.

Chapter 4

Definition of the model

This chapter presents an overview of the model used for describing wetland environments. The partial differential equations (PDEs) involved are the Navier-Stokes equations for the hydrodinamic model and advective-diffusion equation for the solute transport model. The objective is to define the stresses and the breakdown rate due to vegetation as function of its intensity and its diameter. These equations are derived showing the most common model of closure used to treat spatial and temporal irregularities of the main variables with a particular attention on mixing processes over two dimensional domains. At the end of the chapter, there is a brief description of the numerical method used for solving these partial differential equations.

4.1   Hydrodynamic model

The Navier-Stokes equations are the basic governing equations for a real viscous fluid. They are obtained by applying Newton's Law of Motion to a fluid element and it is also called the momentum equation. The 2D Navier-Stokes equations for a weakly compressible (ρ=constant) fluid are:

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0 \qquad (4.1)$$

$$\frac{\partial u_x}{\partial t} + u_x\frac{\partial u_x}{\partial x} + u_y\frac{\partial u_y}{\partial y} = \frac{1}{\rho}F_x - \frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{1}{\rho}\frac{\partial \tau_{xx}}{\partial x} + \frac{1}{\rho}\frac{\partial \tau_{xy}}{\partial y} \tag{4.2}$$

$$\frac{\partial u_y}{\partial t} + u_x\frac{\partial u_y}{\partial x} + u_y\frac{\partial u_y}{\partial y} = \frac{1}{\rho}F_y - \frac{1}{\rho}\frac{\partial p}{\partial y} + \frac{1}{\rho}\frac{\partial \tau_{yx}}{\partial x} + \frac{1}{\rho}\frac{\partial \tau_{yy}}{\partial y} \tag{4.3}$$

where u_x and u_y are the instantaneous velocity components along x and y direction [L/T], p is the pressure [F/L^2], ρ is the water density [M/L^3] and τ_x^v and τ_y^v[F/L^2] account for the total resistance along x- and y- direction. These equations can be rewritten for a spatial domain Ω with boundary $\partial\Omega$, assuming stationary condition hydrostatic pressure and neglecting the Coriolis acceleration and the wind stresses [*Wu et al.* (2005)]:

$$\frac{\partial(hU)}{\partial x} + \frac{\partial(hV)}{\partial y} = 0 \tag{4.4}$$

$$\frac{\partial(hU^2)}{\partial x} + \frac{\partial(hUV)}{\partial y} = -gh\frac{\partial z_s}{\partial x} - \frac{\tau_{bx}}{\rho} - \frac{\tau_{vx}}{\rho} \tag{4.5}$$

$$\frac{\partial(hUV)}{\partial x} + \frac{\partial(hV^2)}{\partial y} = -gh\frac{\partial z_s}{\partial y} - \frac{\tau_{by}}{\rho} - \frac{\tau_{vy}}{\rho} \tag{4.6}$$

where the quantities U and V are the time-depth-averaged velocities [L/T] along the x- and y- direction respectively, h is the water depth [L], z_s is the water surface elevation [L]. The terms τ_x^b and τ_y^b account for bed resistance, whereas τ_x^v and τ_y^v account for vegetation resistance along the x- and y- direction, respectively. In the previous equations Reynolds stresses are neglected, in fact it has seen based on the laboratory studies that the contribution of the Reynolds stresses is generally negligible, compared to the contribution given by the bed roughness and vegetation resistance.

The bed stresses assume the form proposed by [(*Kadlec*, 1990)]:

$$\tau_x^b = \rho c_D^b U\sqrt{U^2 + V^2} \tag{4.7}$$

$$\tau_y^b = \rho c_D^b V \sqrt{U^2 + V^2} \tag{4.8}$$

where c_D^b [-] combines both laminar and turbulent stresses as follows [(*Kadlec*, 1990)]:

$$c_D^b = \frac{3\mu}{\rho h \sqrt{U^2 + V^2}} + f^2 g h^{-1/3} = \frac{3}{Re_h} + f^2 g h^{-1/3} \tag{4.9}$$

The term μ is the dynamic viscosity [M/LT] and f the Manning's friction coefficient [$T/L^{1/3}$]. For low depth-Reynolds numbers the first term representing laminar condition dominates,while for high depth-Reynolds numbers representing turbolent condition, the second term takes over [*Kadlec* (1990)].

For considering vegetation resistance a drag formulation is laso used and the vegetation is modeled as an array of randomly distributed cylinders with uniform diameter d [L] (representing the steams), as suggested by [*Kadlec* (1990)] and by [*Arega and Sanders* (2004)]:

$$\tau_x^v = \frac{1}{2}\rho c_D^v \mu l d U \sqrt{U^2 + V^2} \tag{4.10}$$

$$\tau_y^v = \frac{1}{2}\rho c_D^v \mu l d V \sqrt{U^2 + V^2} \tag{4.11}$$

where μ is the superficial stem density [$1/L^2$], l is the submerged stem length [L] and c_D^v the vegetation drag coefficient. For completely emergent vegetation, as modeled in this case, the submerged stem length can be regarded as the water depth.

Behavior of the vegetation drag coefficient for a singular cylinder under different flow conditions, described by the stem Reynolds number $Re_d = \sqrt{U^2 + V^2} D/\nu$ is well established [*White* (1991)] and shows a decreasing trend as Re_d increases. Additionally, other past and recent studies [*Petryk* (1969); *Nepf* (1999)] show an influence of neighboring cylinders that can produce a velocity deficit and a consequent reduced drag [*Tanino and Nepf* (2008)]. Nevertheless, cumulative effects

of multiple wake interaction can be discarded for sufficiently sparse vegetation distributions, that is when solid volume fraction **a**$d < 0.1$ [*Raupach* (1992)]. The term **a** represents the frontal area of vegetation per unit volume [$1/L$] that can be rewritten, if the plants are modeled by cylinders, as a function of superficial stem density, **a** $= nd$. [*Nepf* (1999)].

Numerical and laboratory experiments showed ralatively constant values of c_D^v up to **a**$d \approx 0.01$ (i.e. $nd^2 \approx 0.01$) that holds to a value of superficial stem density <2500 stems/m^2 if a stem diameter of $2mm$ is chosen.Such values are common in natural and constructed wetlands: [*Tanner* (2001)] measured superficial densities of 1400-1500 stems/m^2 of *Schoenoplectus Tabernaemontani* and >2000 stems/m^2 of *Schoenoplectus Validus* in pilot-scale constructed wetlands whereas found superficial vegetation density of *Phragmites Australis* ranging between 70-250 stems/m^2. Other hydraulic studies on diffusion in emergent vegetation [*Nepf* (1999)] and vegetation drag [*Hall and Freeman* (1994)] used densities ranging between 200-2000 stems/m^2 and 400-800 stems/m^2.

In this study, a vegetation density range between 400 and 2800 stems/m^2 was investigated, allowing the choice of a vegetation drag coefficient dependent only on stem Reynolds number. To model a continuous range of stem Reynolds numbers, the relationship proposed by [*Kadlec* (1990)] observing laboratory tests performed by Wieselberger1921 for laminar flow and Tritton1959 for turbulent flow, was chosen. Kadlec's formulation, similar to that proposed by [*White* (1991)], is:

$$c_D^v = \frac{10\mu}{\rho D \sqrt{U^2 + V^2}} + 1 = \frac{10}{Re_d} + 1 = \frac{10}{Re_h}\frac{h}{D} + 1 \qquad (4.12)$$

4.2   Solute Transport Model

The transport of mass of fluid considered is affected by two different processes: advection and diffusion.

The flux of mass repressnts the sum of these two contributes and it can be written in this form:

$$\phi = \mathbf{u}c - D_m \nabla c \tag{4.13}$$

The first term is the convective component with $\mathbf{u} = (u, v, w)[L/T]$ velocity vector field and c [M/L^3] the mass of the dissolved substance per unit volume.

The second term is the diffusive component, related to the transfer of mass due to the Brownian motion, which says that as a matter of probability there is mass transport from zones characterized by high concentrations to zones characterized by low concentrations. This component is defined by Fick's law, which assumed that the net mass flux of solute is given by the product of the concentration gradient and the molecular diffusion coefficient D_m [L^2/T], under the assumption of steady state. The molecular diffusion coefficient is a constant, and it depends on solute and solvent features. In water environments, molecular diffusion is of the order of $10^{-8} \div 10^{-10}$ m^2/s. Of course the diffusive contribute must be considered negative, in fact this component acts reducing the concentration gradient.

At this point considering a control volume and making a balance of the incoming and outcoming flux it is possible to define the variation of mass inside the volume. Then the advective diffusion equation considering a first order decay can be written as:

$$\frac{\partial c}{\partial t} = -\nabla(\mathbf{u}c - D_m \nabla c) + \lambda c \tag{4.14}$$

where λ [1/T] is the decay rate. Generally a wetland has turbuent flow, hence, due to the unpredictable nature of turbulence requires that we describe the motion through statistical measures. The velocity and the concentration will be de-

scribed as a time-averaged values ($\overline{u}$, $\overline{c}$) plus some fluctuations (u', c'):

$$u = \overline{u} + u' \tag{4.15}$$

$$c = \overline{c} + c' \tag{4.16}$$

where the time-averaged velocity and concentration are defined as:

$$\overline{u} = \frac{1}{T} \int_T u \, dt \tag{4.17}$$

$$\overline{c} = \frac{1}{T} \int_T c \, dt \tag{4.18}$$

Sobstituting the instant velocity and concentration with time-averaged and fluctuation terms, neglecting the molecular transport that is generally much lower than the turbulent transport, with the assumption of incompressible fluid and integrating on the depth, it obtains the final equation that will be used for the transport model:

$$\frac{\partial(hC)}{\partial t} + U\frac{\partial(hC)}{\partial x} + V\frac{\partial(hC)}{\partial y} = \frac{\partial}{\partial x}(hE_x\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(hE_y\frac{\partial C}{\partial y}) + h\lambda C \tag{4.19}$$

where C is the depth-averaged solute concentration $[M/L^3]$, U, V are the vertically integrated velocity components $[L/T]$ in the x-, y- directions respectively. Coefficients E_i, ($i = x,y$) $[L^2/T]$, account for both turbulent diffusion and dispersion. The dispersion effect arises from the non-uniform distributions of flow velocity and solute concentration over the flow depth. *Nepf* (1999) proposed for the horizontal diffusivity the following relationship:

$$\frac{E_T}{Ud} = \alpha_1[c_D^v\mathbf{a}d]^{1/3} + \frac{\beta^2}{2}\mathbf{a}d \tag{4.20}$$

The first term represents the turbulent diffusivity and the second term describes the effect of mechanical diffusion that reflects the dispersal of solute particles caused by different flow paths through stem population. Coefficients $\alpha_1 = 0.81$ [-], derived by *Nepf* (1999) from experimental data, accounts for horizontal turbulent diffusion and coefficient $\beta = 1$ [-] represents a scale factor that takes into account the transversal motion of a solute particle through stems at a distance $\Delta y = \beta d$. Turbulent diffusivity is obtained assuming that all the energy extracted from the mean flow through stems is converted in turbulent kinetic energy. This assumption holds below $Re_d < 200$, where the viscous drag becomes increasingly important.

As showed by Nepf's experiments, for a sufficiently small stem densities, that is for $\mathbf{a}d < 0.01$, mechanical diffusion is small compared to turbulent diffusion and therefore the second term can be neglected. Experiments, performed considering stem Reynolds numbers ranging between 90 and 2000 (typical value ≈ 200 - 300), show that this can not be the case below the lower end of this range for which mechanical diffusion dominates.

Nevertheless, *Lightbody and Nepf* (2006) used this theory, as a first approximation, to determine the longitudinal dispersion coefficient E_L using field velocity measurements ranging between 0.1 and $0.24\,cm\,s^{-1}$ ($Re_d = 2-360$). The purposed longitudinal dispersion coefficient is written as a combination of the stem-scale and of the depth-scale dispersion process as follows:

$$\frac{E_L}{Ud} = \frac{1}{2}c_D^{v\,3/2} + \frac{Uh}{D_z}\Gamma \tag{4.21}$$

where $D_z = \alpha_2[c_D^v \mathbf{a}d]^{1/3}Ud$ is the vertical turbulent diffusion coefficient similar to the first term of eq.4.20 in which a value of $\alpha_2 = 0.1$ was chosen in order to account for the vertical turbulent diffusion and Γ is the non-dimensional velocity shape factor. As described by *Lightbody and Nepf* (2006), the first term, that

describes the stem-scale longitudinal dispersion process, is very small compared to the second one that takes into account the depth-scale dispersion process. The decay rate λ is assumed to be linearly proportional to the stem density.

4.3   Brief description of model resolution of PDEs

For the differential equations previously described it is usually very difficult to obtain solution which explain the behavior of the system. Today thanks to the improvement of computer performances it has become possible to solve these differential equations using numerical techniques.

In this case finite elment method is used. It based on an estimation of a derivative by the ratio of two differences according to a theoretical definition of the derivative. Considering a function $u(x)$, the derivative at a point x is defined as:

$$u_x = \frac{\partial u}{\partial x} = \lim_{\Delta x \to 0} \frac{u(x + \Delta x) - u(x)}{\Delta x} \tag{4.22}$$

Removing the limit in the above equation, it obtains a finite difference, which explains the name given to this method. If Δx is small but finite, the expression on the right-hand side is an approximation to the exact value of u_x. The approximation will be improved by reducing Δx , but for any finite value of Δx, an error is introduced, the truncation error, which goes to zero for Δx tending to zero.

The power of Δx with which this error tends to zero is called the order of accuracy of the difference approximation, and can be obtained from a Taylor series development of $u(x + \Delta x)$ around point x. Actually, the whole concept of finite difference approximations is based on theproperties of Taylor expansions. Developing $u(x + \Delta x)$ around $u(x)$ we have:

$$u(x + \Delta x) = u(x) + \Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3} + \ldots \tag{4.23}$$

that can be written as:

$$\frac{u(x + \Delta x) - u(x)}{\Delta x} = u_x(x) + \frac{\Delta x}{2} u_{xx}(x) + \frac{\Delta x^2}{6} u_{xxx}(x) + ... \tag{4.24}$$

showing that the right-hand side (r.h.s) of equation (4.22) is indeed an approximation to the first derivative u_x in point x, the remaining terms in the r.h.s represent the error associated to this formula.

If it restricts the truncation error to its dominant term, that is to the lower power in Δx, it is possible to see that this approximation for $u(x)$ goes to zero like the first power of Δx and is said to be first order in Δx and it writes:

$$\frac{u(x + \Delta x) - u(x)}{\Delta x} = u_x(x) + \frac{\Delta x}{2} u_{xx}(x) = u_x(x) + O(\Delta x) \tag{4.25}$$

indicating that the truncation error $O(\Delta x)$ goes to zero like the first power in Δx. A very large number of finite difference approximations can be obtained for the derivatives of functions.

Chapter 5

Hydrodinamic analogy

This chapter presents a description of the steps and the assumptions that has been made for obtaining an analogy between the equations that are generally used for modelling 2D shallow water flows and the equations used for the 2D weakly compressible fluids, which are also the equations that Comsol multiphysics solves. In this case it has been considered steady state conditions.

In the first part it is introduced the equations for a weakly compressible fluid, then a description of the equations used for shallow water flow with some assumptions that have been made.

In the second part there is a comparison between the final equations obtained, through which it is possible to make an analogy between the variables involved.

The equations for a 2D weakly compressible fluid considering stationary state can be written as:

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0 \tag{5.1}$$

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{\partial (P)}{\partial x} + \frac{\partial}{\partial x}[(\frac{4}{3}\eta + k_{dv})\frac{\partial u}{\partial x} - (\frac{2}{3}\eta - k_{dv})\frac{\partial v}{\partial y}] + \frac{\partial}{\partial y}[\eta(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})] + F_x \tag{5.2}$$

$$\rho u \frac{\partial v}{\partial y} + \rho u \frac{\partial v}{\partial x} = -\frac{\partial (P)}{\partial y} + \frac{\partial}{\partial y}[(\frac{4}{3}\eta + k_{dv})\frac{\partial v}{\partial y} - (\frac{2}{3}\eta - k_{dv})\frac{\partial u}{\partial x}] + \frac{\partial}{\partial x}[\eta(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y})] + F_y \tag{5.3}$$

where: ρ $[M/L^3]$ is the fluid density, u and v $[L/T]$ are the velocities along x-y directions, p $[M/LT^3]$ is the pressure, η the dynamic viscosity, k_{dv} the dilatation viscosity and F_x, F_y $[F/L^3]$ are the volume forces along x-y directions.

The equation for a 2D shallow water flow considering the stationary state form can be written as:

$$\frac{\partial hu}{\partial x} + \frac{\partial hv}{\partial y} = 0 \tag{5.4}$$

$$\frac{\partial hu^2}{\partial x} + \frac{\partial huv}{\partial y} = -gh\frac{\partial z_s}{\partial x} + \frac{1}{\rho}\frac{\partial hT_{xx}}{\partial x} + \frac{1}{\rho}\frac{\partial hT_{xy}}{\partial y} + \frac{1}{\rho}(\tau_{sx} - \tau_{bx}) + f_c hv \tag{5.5}$$

$$\frac{\partial huv}{\partial x} + \frac{\partial hv^2}{\partial y} = -gh\frac{\partial z_s}{\partial y} + \frac{1}{\rho}\frac{\partial hT_{yx}}{\partial x} + \frac{1}{\rho}\frac{\partial hT_{yy}}{\partial y} + \frac{1}{\rho}(\tau_{sy} - \tau_{by}) + f_c hu \tag{5.6}$$

where: ρ $[M/L^3]$ is the fluid density, u and v $[L/T]$ are the velocities along x-y directions, h $[L]$ is the water level, g $[L/T^2]$ is the gravitational acceleration η the dynamic viscosity, k_{dv} the dilatation viscosity and τ_{sx} and τ_{sy} are the stresses due to wind forces along x-y direction, τ_{bx} and τ_{by} are the stresses due to bed roughness and vegetation along x-y directions and f_c is a Coriolis coefficient. Assuming that for our porposes it is possible to neglect both Coriolis and wind forces, and consideing the following relations:

$$z_s = z_b + h \tag{5.7}$$

$$\frac{\partial z_s}{\partial x} = \frac{\partial z_b}{\partial x} + \frac{\partial h}{\partial x} = -i_x + \frac{\partial h}{\partial x} \tag{5.8}$$

$$\frac{\partial z_s}{\partial y} = \frac{\partial z_b}{\partial y} + \frac{\partial h}{\partial y} = -i_y + \frac{\partial h}{\partial y} \tag{5.9}$$

and that the T_{xx}, T_{xx}, T_{xx} and T_{xx} can be defined as:

$$T_{xx} = 2\rho(\nu + \nu_t)\frac{\partial u}{\partial x} - \frac{2}{3}\rho k \tag{5.10}$$

$$T_{yy} = 2\rho(\nu + \nu_t)\frac{\partial v}{\partial y} - \frac{2}{3}\rho k \tag{5.11}$$

$$T_{xy} = T_{yx} = \rho(\nu + \nu_t)(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}) \tag{5.12}$$

I obtain

$$hu\frac{\partial u}{\partial x}+hv\frac{\partial u}{\partial y} = -ghi_x-g\frac{\partial h^2/2}{\partial x}+\frac{1}{\rho}\frac{\partial}{\partial x}[2h\rho(\nu+\nu_t)]+\frac{1}{\rho}\frac{\partial}{\partial y}[h\rho(\nu+\nu_t)(\frac{\partial u}{\partial y}\frac{\partial v}{\partial x})]-c_f m_b u\sqrt{u^2+v^2} \tag{5.13}$$

where:

$$m_b = [1 + (\frac{\partial z_b}{\partial x})^2 + (\frac{\partial z_b}{\partial})^2]^{\frac{1}{2}} = \sqrt{(1 + i_x^2 + i_y^2)} \tag{5.14}$$

$$c_f = gn^2 h^{-1/3} \tag{5.15}$$

Considering:

- ν_t constant

- parabolic model averaged on the tubrulance

I can write:

$$\nu_t = \alpha U_* h = \alpha\sqrt{\frac{T_0}{\rho}}h \tag{5.16}$$

Where α is defined equal to $k/6$ and U_* is defined considering uniform flow.

From computantion I obtain that I can write:

$$\nu_t = \alpha\sqrt{g}n\sqrt{u^2+v^2}h^{5/6} \tag{5.17}$$

Then the first equation becomes:

$$hu\frac{\partial u}{\partial x} + hv\frac{\partial u}{\partial y} = -\frac{\partial}{\partial x}(g\frac{h^{(2)}}{2}) + \frac{\partial}{\partial x}[2h(v+v_t)\frac{\partial u}{\partial x}]+$$

$$\frac{\partial}{\partial y}[h(v+v_t)(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})] - gn^2h^{-1/3}(1 + i_x^2 + i_y^2)^{1/2}u\sqrt{u^2 + v^2} - ghi_x \tag{5.18}$$

Now we can compare this equation for shallow water flow with the equation for weakly compressible fluid (gas)

$$\nabla(\rho\mathbf{u}) = 0 \tag{5.19}$$

$$\nabla(h\mathbf{u}) = 0 \tag{5.20}$$

We can see that we can assume $h = \rho$

In the same way comparing the other two equations we obtain the following substitutions:

$$\rho = h; \qquad P = \frac{1}{2}gh^2 \tag{5.21}$$

$$K_d = \frac{2}{3}\eta; \qquad \eta = (v + v_t)h \tag{5.22}$$

Riproduction of vegetated fields

This chapter presents a description of the code and the steps followed for generating a serie of random fields, for modeling the vegetation distribution of some wetlands, including some statistical features. The created fields will be used as input, for the resolution of the hydrodinamics model and the solute transport model. For the creation of these fields HydroGen program is used [*Bellin and Rubin* (1996)].

6.1   Introduction to HydroGen algorithm

HydroGen is an algorithm developed for generating spatially-correlated random fields which well represent the natural heterogeneity and spatial variability encountered in the hearth sciences. The method is based on two obsevations: spatially distributed attributes usually display a stationary correlation structure and the screening effect of measurements leads to the sufficiency of a small research neighborhood when it comes to projecting measurements and data in space.

6.2 Mathematical statement of the problem and field generation technique

6.2.1 General approach

Consider a spatially distributed attribute $z(x)$, where x denotes the spatial coordinate. In order to model its spatial structure, $z(x)$ is modeled as a space random function (SRF) $Z(x)$. $Z(x)$ is characterized statistically by its moments, for example its expected value:

$$\langle (x) \rangle = m_z(x) \tag{6.1}$$

and its spatial covariance:

$$C_Z(x, x') = \langle [Z(x) - m_z(x)][Z(x') - m_z(x')] \rangle = C_Z(r = x - x') \tag{6.2}$$

In case $Z(x)$ is either Gausian or log-Gaussian, its etire distribution is defined by 6.1 and 6.2. In this case only Gaussian Z has been considered. Note that for $x = x'$, $C_Z(x, x) = \sigma_Z^2(x)$ is the variance of Z, which must be finite to ensure that the covariance is well defined. In the case of an infinite variance, $Z(x)$ cannot be defined through its covariance. An alternative [*Journel and Alabert* (1989)] is to define Z through the spatial structure of the increments $Z'(x) = Z(x) - m_z(x)$. The increments are defined by a stationary mean.

$$\langle Z(x) - m_z(x) \rangle = 0 \tag{6.3}$$

and the semivariogram:

$$\gamma_Z(x, x') = \frac{1}{2} \langle [Z'(x) - Z'(x')]^2 \rangle \tag{6.4}$$

The two models above define fields of completely different nature. Equations 6.1 and 6.2 define fields whose heterogeneity is chracterized by a finite integral scale. This model is analogous to one defined by equations 6.3 and 6.4 only when $\gamma_Z(x, x')$ reaches a sill, at a finite separation distance. When the semivariogram γ_Z does not reach a sill, a finite length scale cannot be defined. This type of variability arises in the presence of an infinite sequence of evolving scales of variability. Semivariograms6.4 that scale as $\gamma_Z(r) = ar^{2H}$, $r = \|r$, and $0 < H < 1$, represent self-similar or fractal fields.

The algorithm HydroGen aims at generating replicates of Z fields whose spatial statistics are defined either by 6.1 and 6.2 or alternatively by 6.3 and 6.4. While Z is generally a continuous function, the proposed algorithm consists in generating the Z field discretely over a pre-determined arbitrary grid (.....figure1). The grid can be of variable density and of arbitrary geometry. In the following section, the generating technique for producing a single replicate of Z field is described.

6.2.2   Field generating technique

Consider the determination of Z at x_0 in a field defined by 6.1 and 6.2, where local data are not available. Choosing x_0 to be our starting point, a realization $z(x_0)$ is generated using a standard random generator with the unconditional mean $m_z(x)$ and the unconditional variance σ_Z^2 used as target statistics. Once $z(x_0)$ is generated, it is considered as a datum and it will be used to condition the z values which will be generated subsequently at neighboring nodes. At the next step, generation of a realization at a nearby point x_1 is considered. This time $Z(x_1)$ is conditioned on the previously generated$z(x_0)$, using the Gaussian conditioning procedure [*Mood et al.* (1963)]. The conditional mean is given by:

$$\langle Z^c(x_1) \rangle = m_z(x_1) + \lambda(x_1)[z(x_0) - m_z(x_0)] \tag{6.5}$$
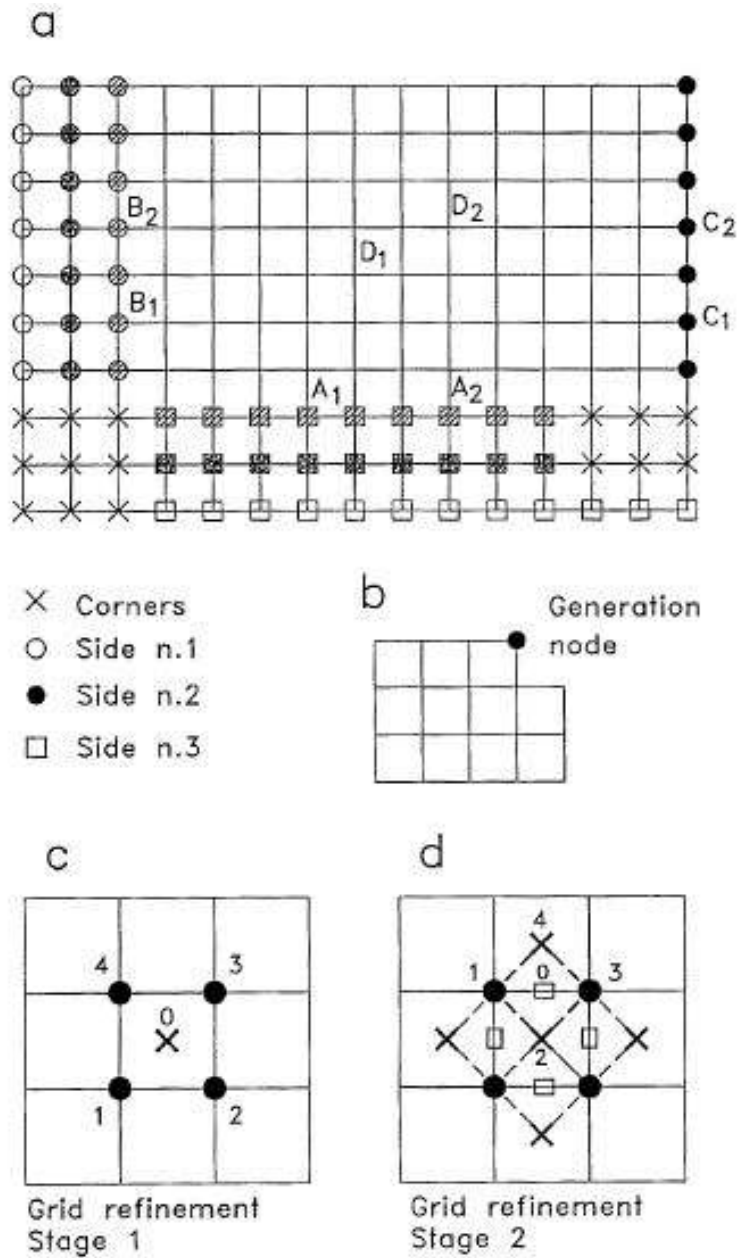
Figure 6.1. Example of domain discretization and grid refinement; a) the coarse grid generation; b) the search neighborhood; c) the first stage refinement; d) the second stage refinement

and the conditional variance by:

$$\sigma_Z^{2c}(x_1) = \sigma_Z^2 - \lambda_1(x_1)C_Z(x_1, x_0) \tag{6.6}$$

Here and subsequently superscript c denotes "conditional". The cofficient $\lambda(x_1)$ is given by [*Dagan* (1989)]:

$$\lambda_1(x) = \frac{C_Z(x_0, x_1)}{\sigma_Z^2} \tag{6.7}$$

Once $\langle Z^c(x_1) \rangle$ and σ_Z^{2c} are determined, a realization $z(x_1)$ for $Z(x_1)$ is generated based on these target statistics and is also added to the data base for conditioning at later steps. In the more general case it generates a realization for a generic $Z(x_N)$, using the previously generated $(N-1)$ data at $(N-1)$ nodes for conditioning. The conditional axpected value of $Z(x_N)$ is given by:

$$\langle Z^c(x_N) \rangle = m_z(x_N) + \sum_{j=1}^{N-1} \lambda_j(x_N)[z(x_j) - m_z(x_j)] \tag{6.8}$$

while the conditional variance is given by:

$$\sigma_Z^{2c}(x_N) = \sigma_Z^2 - \sum_{j=1}^{N-1} \lambda_j(x_N)C_Z(x_N, x_j) \tag{6.9}$$

Once these last two statistics are computed, $s(x_N)$ can be generated from any standard generator which uses these two statistics as target statistics. The steps applied to the generic x_N are repeated for all designed nodes. The only difference between consecutive steps is in the number of data used for conditioning and hence of the number of interpolation coefficients which keeps increasing. The coefficient λ_j (equations 6.8, 6.9) are the solution of the following linear system

[*Dagan* (1989)]:

$$\sum_{j=1}^{N-1} \lambda_j(x_N)C_Z(x_j,x_q) = C_Z(x_N,x_q); \qquad q = 1,....,N-1 \qquad (6.10)$$

In matrix notation the system 6.10 is written as:

$$A\Lambda = \sum \qquad (6.11)$$

where the matrix of coefficients A is given by

$$A = \begin{pmatrix} C_Z(x_1,x_1) & \cdots & C_Z(x_1,x_{N-1}) \\ C_Z(x_j,x_1) & \cdots & C_Z(x_j,x_{N-1}) \\ C_Z(x_{N-1},x_1) & \cdots & C_Z(x_{N-1},x_{N-1}) \end{pmatrix}$$

Λ is thee vector containing the interpolation coefficients:

$$\Lambda = [\lambda_1(x_N),...,\lambda_{N-1}(x_N)] \qquad (6.12)$$

Finally, the vector $\sum$ is defined by:

$$\sum = [C_Z(x_N,x_1),...,C_Z(x_N,x_{N-1})] \qquad (6.13)$$

The repetitive solution of 6.11 (i.e., for each new node) is computationally the most demanding step in the algorithm. The order of the matrix $A6.2.2$ grows linearly with N and its repetitive inversion for each new x_N can slow down considerably the computations. Since the purpose of HydroGen is to generate numerous independent replicates of the Z field at low computational cost, this aspect of the algorithm can turn into a major obstacle, and hence is addressed here further. The computational effort associated with the inversion of the algorithm can be

alleviated significantly when considering the following points:

- The integral scale of Z is finite, resulting from the rapid decay of the covariance $C_Z(r)$;

- The interpolation coefficients λ_j (6.8) associated with any node x_j do not depend on the actual values of $z(x_j)$ at the surrounding nodes but rather on the distances $x_k - x_j$, $k = 1,...,N-1$ [*Journel*]. As a result, $Z(x_N)$ needs to be conditioned only on a limited search neighborhood, and furthermore, if a fixed-size search neighborhood with a fixed spatial configuration of conditioning data is used, the set of coefficients Λ (6.12) needs to be computed once and only once and can then be used repeatedly for any x_N.

A salient question is the size of the search neighborhood. This question was resolved in our study through extended numerical axperimentation. From a practical point of view, however, the previous observations dictate that the "filling-in" of the Z values over the grid should be carried out in a way that allows using fixed sets of interpolating coefficients. The HydroGen concept can now be presented as an algorithm with the following steps (referring to a generic point x_N, and given the data set of all the previously generated z_j, $j < N$):

- Compute $\langle Z^c(x_N) \rangle$ and $\sigma_Z^{2c}(x_N)$, conditional to all data at points contained inside of the search neighborhood, using equations (6.8) and 6.9. The shape of the search neighborhood resembles the letter "L" with x_N placed inthe upper right corner (see Figure 1b).

  The characteristic dimension of the search neighborhood, r_s is the larger side of the above rectangle. For isotropic fields the rectangle is transformed into a square of dimension r_s. figure 1a shows with different symbols the zones of domain characterized by the same set of interpolation coefficients. the generation of Z at the nodes D_1 and D_2 in Figure 1a as well as that at the unmarked nodes are obtained using the same set of interpolation cofficients which are computed using all the nodes of the search neighborood shown

in Figure 1*b*. Other sets of interpolation coefficients are used to generate the field at nodes A_1 and A_2 as well as at all nodes indicated by shaded boxes. Similar considerations can be done for the other zones indicated by symbols in Figure 1*a*. For example, $C_!$ and C_2, or $B_!$ and B_2 require the same set of coefficients.

- Generate a realization $z(x_N)$ using the conditional mean and variance computed at the previous step as target statistics.

- Add $z(x_N)$ to the data base for conditioning of $z(x_{N+1})$, with x_{N+1} being the next node.

- Move to next node according to an a-priori determined scheme, increase N by 1, and go up to the first step.

The data used for conditioning can be of two types: realization of $Z(x_i), i < N$, which were generated at the previous step, and actual field data. When data of the first and second type are used, the generated fields are said to be conditional fields, meaning that the spatial statistics are constructed, and that the generated fields are constrained by measurements.

When the first replicate of the Z-field is constructed, there is a need to recompute a set of interpolating coefficients (6.12) for new data configuration when moving along the grid's periphery. On a regular grid the pattern most economical from a computational point of view is to generate z values along rows, moving row by row (or column by column). This method is similar to the Sequential Simulator method by Gomez-Hernandez and Srivastava.

Both methods condition on generated Z values contained within a suitable search neighborood when generating the actual value of $\langle Z^c(x_N) \rangle$ at x_N. The actual value of Z is then computed by a Gaussian random generator using $\langle Z^c(x_N) \rangle$ and $\sigma_Z^{2c}(x_N)$ at the point x_N. The two methods differ in the following aspects: while the Sequential Simulator Method uses different paths to fill in the values

of Z for different realizations, this method uses a fixed pattern for all the realizations. Using a fixed pattern leads to a dramatic reduction in the requirements. The saving in CPU time become very significant when a large number of fields are generated. The use of a fixed pattern is made possible by the reliance on a relatively large search neighborhood. The benefits from the initial investment in computing a few sets of interpolation coefficients is in the ability to produce an enormous number of replicates at negligible computational cost.

6.2.3   Multi-stage grid refinement

The density of the grid (Figure 1) bears significantly on the computational burden and needs to be considered carefully prior to any application. Generally, high density grid implies an increase in the computational burden, both at the field generation stage and also when it comes to application of the transfer function, yet it is often necessary in order to ensure sufficient resolution of the dependent variables produced by the tranfer function. For example, in order to correctly simulate contaminant transport in highly heterogeneous geologic formations, a high level of discretization of the conductivity field is required.

However, an advantage may be takenfrom the fact that the high resolution is needed only over the portions of the simulated domain which are actually "visited" by the plume. To allow for high, spatially variable resolution, this method introduces multi-stage grid refinement. The grid can be refined to any a-priori determined level of discretization, and the refinement can be executed over any subset of the grid as a dictated by the problem.

Grid refinement is performed as follows. First, realizations of Z at the nodes of a coarse initial grid obtained following the methodologyoutlined in section 6.2.2. Then, subsections of the grid are refined by increasing the density of nodes. Since large-scale spatial correlation is already taken care of at an early stage, the additional Z values are computed using (6.8), but conditioned only on the nearest

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neighbors, thus utilizing the screening effect often employed in geostatistical applications. Figure 1c and 1d show an example of refinement for a generic coarse grid cell.

The refinement consists in two steps. First, a realization of Z at the cell's centre is generated conditional to the Z values at the four coarse grid neighborhood points marched by [●] on Figure 1c. This step is followed by the generation of Z values at the four nodes on the cell boundaries marked by [◇] on Figure 1d. This is accomplished by conditioning on the four closest nodes simmetrically located around the node under consideration. Figure 1d shows an example of second stage refinement.

According to the refinement procedure the generation at the node "0" is performed conditioning on nodes indicated by the numbers "1", "2", "3" and "4". The desired level of refinement can be obtained by applying iteratively the above two stage refinement. The computational burden required for generation of a large scale, fine grid field is alleviated by using the multi-stage approach which saves the need for inversion of huge matrices. Furthermore, by refining the grid in a systematic manner, and working with fixed spatial data configurations for the conditioning set, the additional effort becomes pratically nil, since all it takes is one time inversion of a small matrix for each level of refinement.

The HydroGen method is suitable for irregular and non-rectangular grids.Hydrogen can be apllied by first generating the field on a rectangular regular grid, the screening effect ensures that the extra values can be obtained by conditioning on a small search neighborhood. This procedure is advantageous compared to polynomial interpolation since it does not introduce any unnecessary smoothing.

6.2.4   Additional theoretical considerations

It has been discussed so far the case of Z with a known, yet nonstationary axpected value and a stationary covarisnce. The previously outlined approach can

be extended to other models of Z without losing any of its robustness, by using the same principles and modifying the kriging system. The method can be applied to:

- a weakly stationary Z with an unknown mean [*Journel*];

- a weakly stationary Z defined by a semivariogram [*Bras and Rodriguez-Iturbe* (1985)];

- a weakly stationary Z where Z is an intrinsic random function, of order k, where k is a positive integer [*Bras and Rodriguez-Iturbe* (1985)]

When the expected value of Z is nonstationary, the proposed procedure can be applied just the same for the Z residuals $Z' = Z - \langle Z(x) \rangle$, and the generated deviates should be added to the mean. The common aspect to all these models is that the interpolating coefficients depend on the separation distances only.

A particularly interesting case occurs when Z is defined by an unbounded semivariogram. In that case, Z is correlated over aany distance hence a finite search neighborhood which is smaller than the simulated domain cannot be defined. Consequently, aset of coefficients needs to be computed anew for each point. Nevertheless, an economy in the computations is still achieved since the set of the interpolation coefficients are computed only once, during the production of the first replicate. Once the coarse grid generation is completed the multi-stage refinement follows which allows the reduction of the grid spacing to the desired discretization. The long range correlation structure is obtained from the coarse grid generation while the small scale variability is obtained at the refinement stage.

The computational cost decreases as the coarse grid spacing increases as the coarse grid spacing increases. However, to reproduce the long range correlation structure is obtained at the refinement stages. However, to reproduce the long range correlation structure, the coarse grid spacing should not exceed the limit

of 1 to $2I_Z$. The theoretical basis for the ability of the method to produce the prescribed statistics needs further clarification. It defines any of the one point statistics as S (e.g. mean, variance). Its conditional mean is $\langle S(x)|(N_x)\rangle dx$, where $(N_x) = (z_1, z_2, ...z_N)$ is the set of all data contained in the search neighborhood. The spatial average of $\langle S(x)|(N_x)\rangle$ over the entire domain Ω is $\frac{1}{A}\int_\Omega \langle S(x)|(N_x)\rangle dx$, where A is the area of Ω. Due to stationarity:

$$\frac{1}{A}\int_\Omega \langle S(x)|(N_x)\rangle dx = \int_{Z_1}\int_{Z_2}...\int_{Z_N} \langle S(x)|(N_x)\rangle f_{Z_1,Z_2,...,Z_N}(z_1,z_2,...z_N)dz_1...dz_N = \langle S(x)\rangle$$

(6.14)

That is, spatial averaging of the conditional statistics leads to the unconditional, prescribed ones and ergodicity holds. The spatial average of the covariance between any two points with a fixed separation distance r is given by:

$$\frac{1}{A}\int_{\Omega,|x-x'|=r} \langle Z'(x)Z'(x')|N_{x,x'}\rangle dx dx'$$

(6.15)

wher $Z'(x) = Z(x) - \langle Z(x)\rangle$ and $N_{x,x'}$ is the set of points used to condition the covariance. Following again the procedure outined in the previous equation and invoking ergodicity, it is found thet spatial averaging 6.15 is analogous to deconditioning and it leads to reproduction of the theoretical, prescribed covariance.

6.3   Field Generation

At this point it is necessary for creating the fields representing the vegetation distribution to set the statistics of the vegetation that it wants to reproduce. First it has to be fixed the field geometry and the discretization step, then the mean $\mu[1/m^2]$, and the variance $\sigma^2[1/m^4]$ which represents a measure of how far the density of steams is spread out from the mean.

They are defined as:

$$\mu = \frac{1}{A} \int_A x \, dA \qquad (6.16)$$

$$\sigma^2 = \frac{1}{A} \int_A (x - \mu)^2 \, dA \qquad (6.17)$$

where $\mu[1/m^2]$ is the punctual density that has to be integrated in the area $A[m^2]$. For each value of mean different variances have to be chosen. Due to the Gaussian distribution of the densities, for not obteining negative values, that it would have no physical meaning, all the variances have been set respecting the following relationship:

$$mean - 3\sqrt{var} > 0 \qquad (6.18)$$

The last parameters that must be set are: the correlation length $lc[m]$, that is the measure of how the value of the density at a certain point is correlated to the values nearby, and the seed number, which represents the starting point for generating the random fields.

For this work, two rectangular geometries with different dimensions have been considered. The first one for better representing the real wetland dimensions and the real resident time, while the second one allows to use a larger range of mean values. This, because the resolution of the model for the first geometry considering higher values of mean densities, resuts to be too slow.

Geometry 1

First it was considered a rectangular geometry field of length $400m$ and width $300m$, with step equal to $1m$ in both x-y directions. For the mean, three different values were set in a range between 300-1300 $stem/m^2$.

To each mean, different values of variance were associated respecting the relations previously reported. For each couple of these parameters, correlation lengths in a range between 5 and $45m$ were set. Finally three different seed numbers were considered. For this geometry a set of 128 vegetated fields with

different distribution were generated.

Geometry 2

Second it was considered a rectangular geometry field of length 120m and width 90m, with step equal to 1m in both x-y directions. For the mean, five different values were set in a range between 1200-2800 $stem/m^2$.

To each mean, different values of variance were associated respecting the relation previously reported. For each couple of these parameters, correlation lengths in a range between 3 and 15m were set. Only one seed numbers were considered. For this geometry a set of 60 vegetated fields with different distribution were generated.

6.3.1 Examples of vegetation distribution fields
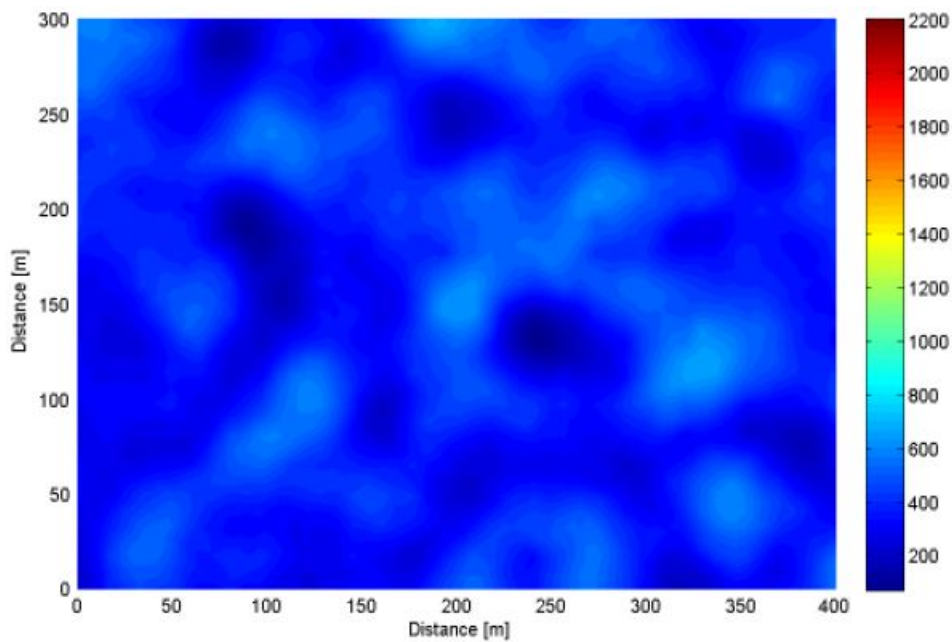
Figure 6.2. Example of random distributed vegetation field with the following statistics: $\mu = 400[m^{-2}]; \sigma^2 = 10000[m^{-4}]$; lc= 25[$m$]; seed number=10000.
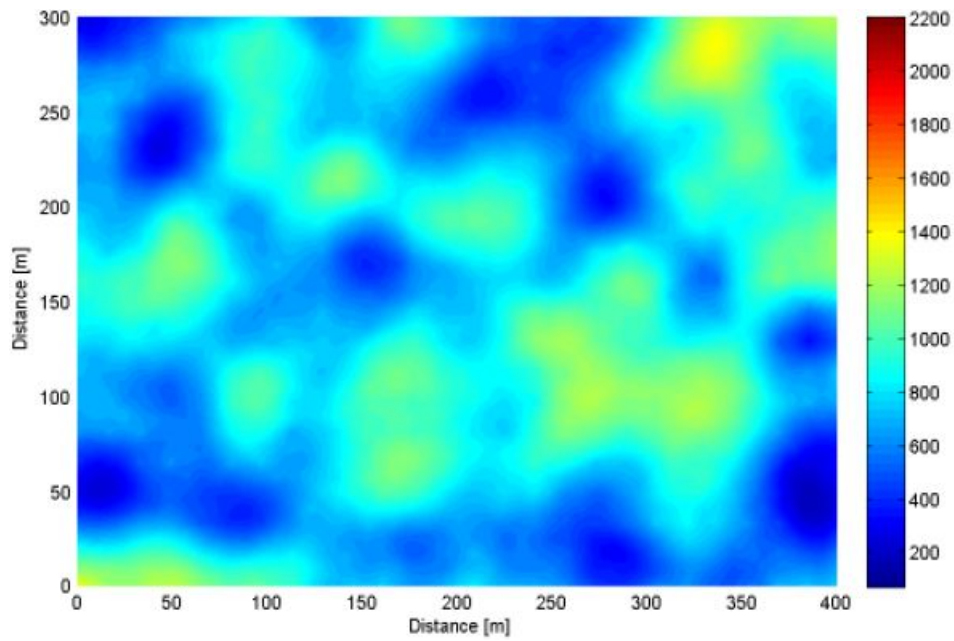
Figure 6.3. Example of random distributed vegetation field with the following statistics:

$\mu = 800[m^{-2}]; \sigma^2 = 40000[m^{-4}]$; lc= 30[m]; seed number=2.
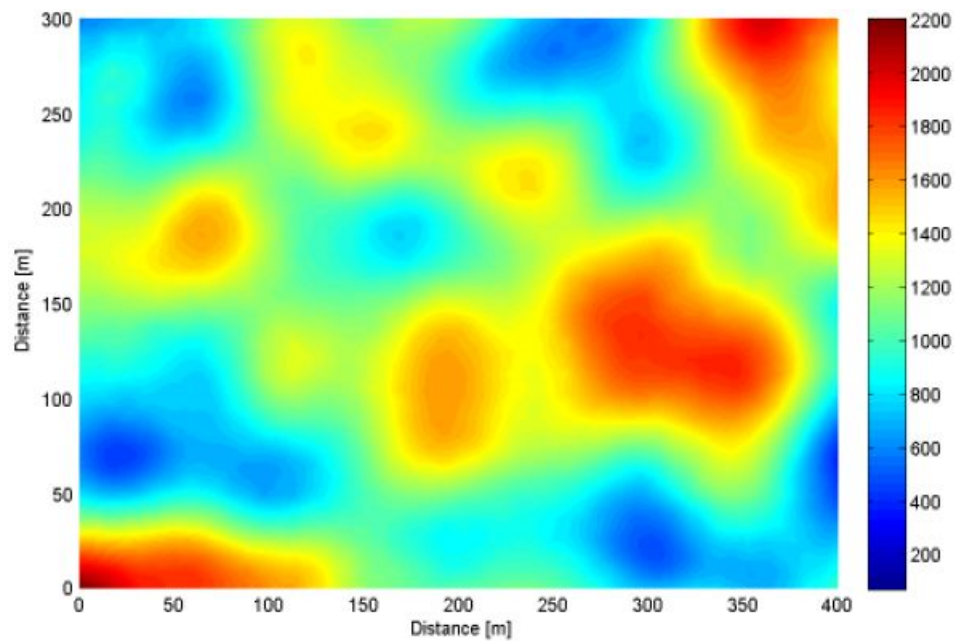
Figure 6.4. Example of random distributed vegetation field with the following statistics:

$\mu = 1200[m^{-2}]; \sigma^2 = 90000[m^{-4}]$; lc= 45[m]; seed number=2.

Chapter 7

COMSOL Multiphysics

This chapter reports a brief description of the COMSOL Multiphysics software that has been used to define and solve the model. It also reports all the constants and the functions which needs to be set up. Finally some examples of otputs referring to different vegetation distribution are inserted.

7.1 Introduction to COMSOL

COMSOL Multiphysics is a powerful interactive environment for modeling and solving all kinds of scientific and engineering problems, based on partial differential equations (PDEs). With this software it is possible easily extend conventional models for one type of physics, into multiphysics models that solve coupled physics phenomena - and do so simultaneously.

In this particular case Solute Transport Model and Hydrodynamic model are combined together.

The first step is to choose the partial differential equations that govern the problem, it is interested in. After this part, it needs to be defined the spatial domain Ω and then specify the boundary functions, the constants and the boundary conditions, related to the problem it has to be solved. Hence it has to be define a mesh. This step is really important in fact, a too large mesh can lead to big errors on the

solution, while a small mesh can lead to a too long time for the resolution of the model. At the end before to solve the model the numerical method for solving the partial differential equations must be chosen. Below the assumption made at each step are reported:

- the partial differential equation considered are 2D Navier-Stokes equations for a weakly compressible fluid regardind the hydrodynamics and the advective-diffusion equation regarding the solute transport model;

- two rectangular geometry $400m$ for $300m$ and $120m$ for $90m$ with an inlet and outlet opens of $10m$ located in the middle of the shorter sides.

- the constants set are: the kinematic viscosity $\nu = 1 * 10^{-6} m^2/s$, the gravity acceleration $g = 9.81 m/s^2$, the slope s_x, s_y set equal to 0 in both directions, the stem diameter $D_s = 0.02m$, the Manning's coefficient representing the bed roughness $n = 0.02 s/m^{\frac{1}{3}}$ and the nondimensional velocity shape factor $\tau = 0.1$;

- it has defined a function in space $s(x, y)$ which gives the vegetation density for each point inside the previously defined domain. Then the volume forces $F_x, F_y [N/m^3]$, the diffusion coefficient $D[m^2/s]$ and the reaction rate $R[mol/(m^3 s)]$;

$$(F_x, F_y, D, R) = f(g, s_x, s_y, \rho, \nu, U, u, s(x, y), n, D_s, \tau) \qquad (7.1)$$

where $U[m/s]$ is the absolute value of the velocity, while $u[m/s]$ and $v[m/s]$ are the velocity respect to $x[m]$ and $y[m]$ directions;

- as boundary condition it was set the downstream level at $0.5m$ and all the edges except the intake and outtake as not permeable walls. At this point it wanted to set the head equal to $0.05m$ for the first geometry, and $0.03m$ for the second one. Because COMSOL software has not this option, an iterative

method was used. First, fixing the inlet velocity, solving the model, evaluating the head by make a difference between inlet and outlet level, and then modifing the inlet velocity using bisection iterative method till the error given by the absolute value of the difference between the fixed head and the computed head is less than a predetermined value;

- it has been considered a triangular mesh with P2-P1 element using second-order elements for the velocity components, and linear elements for the pressure. Different dimension of the element has been considered; a denser mesh has been chosen around the intake and outtake where the high gradients of the velocity could lead to a significant error in the solution of the model;
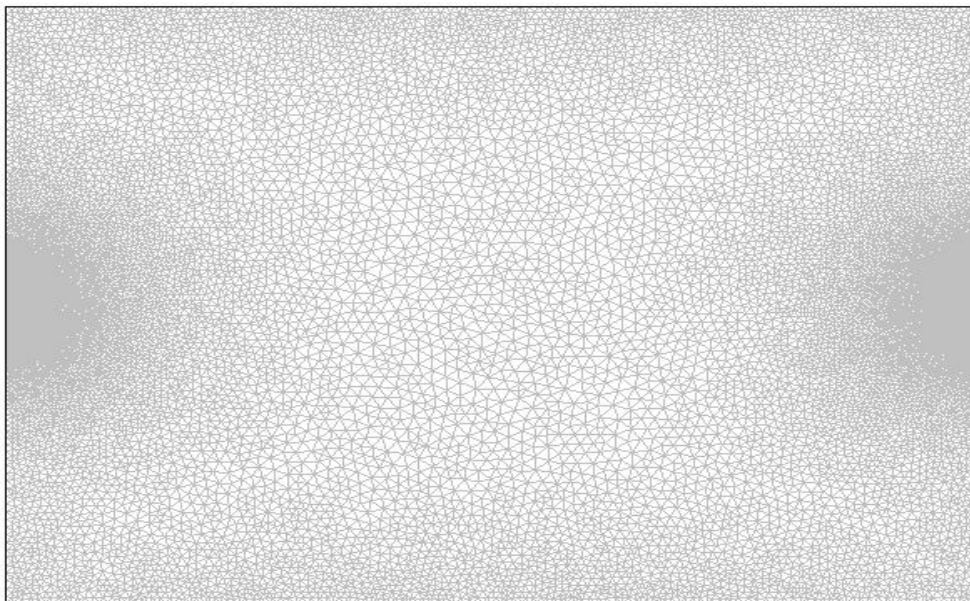
Figure 7.1. Triangular mesh used for solving the model.

- the model is solved using a finite element method briefly described at 4.3.

After solving the model the software gives both numerical and graphical results. Below examples of the results referring to the three vegetation distributions generated in chapter 6.

- These pictures represent the distribution of the absolute velocity:
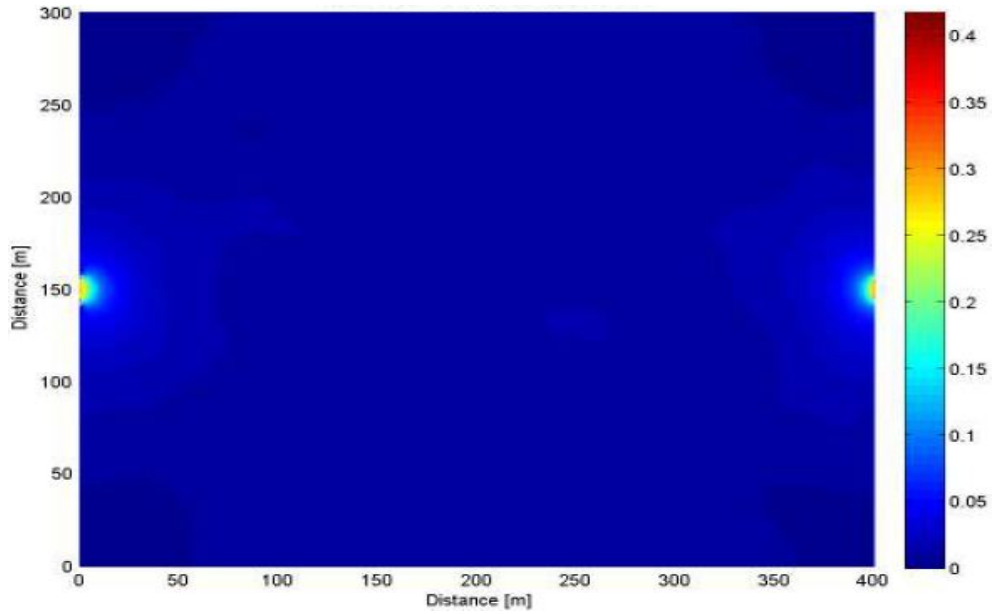
Figure 7.2. Velocity field for distributed vegetation field with the first statistics.
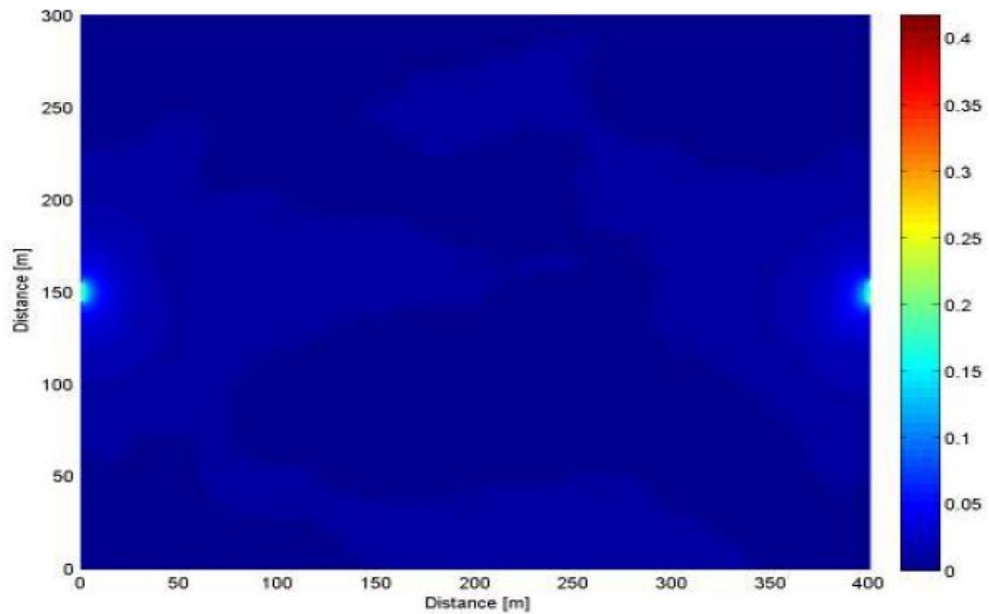
Figure 7.3. Velocity field for distributed vegetation field with the second statistics.
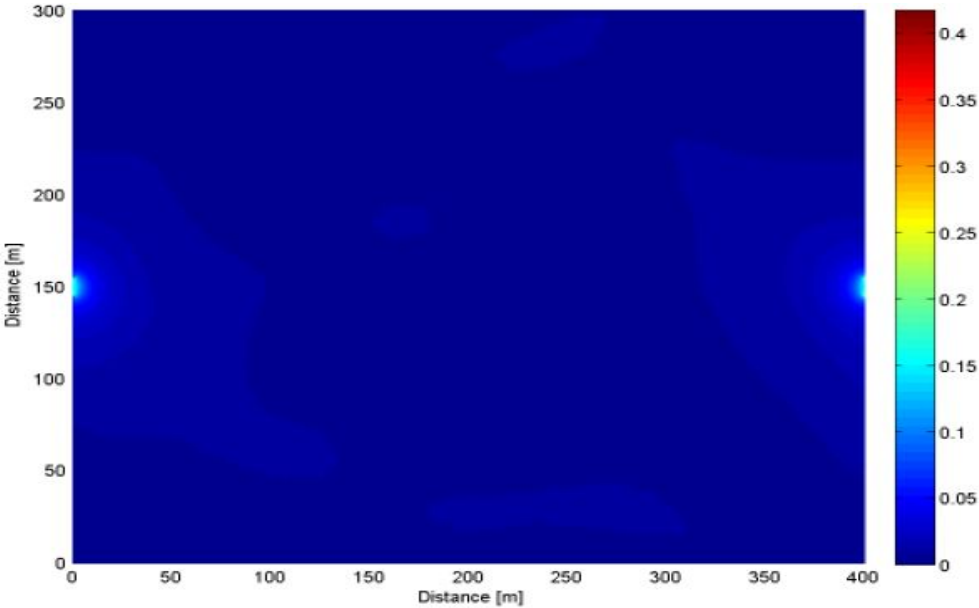
Figure 7.4. Velocity field for distributed vegetation field with the third statistics.

- These pictures represent the distribution of the velocity along x-direction:
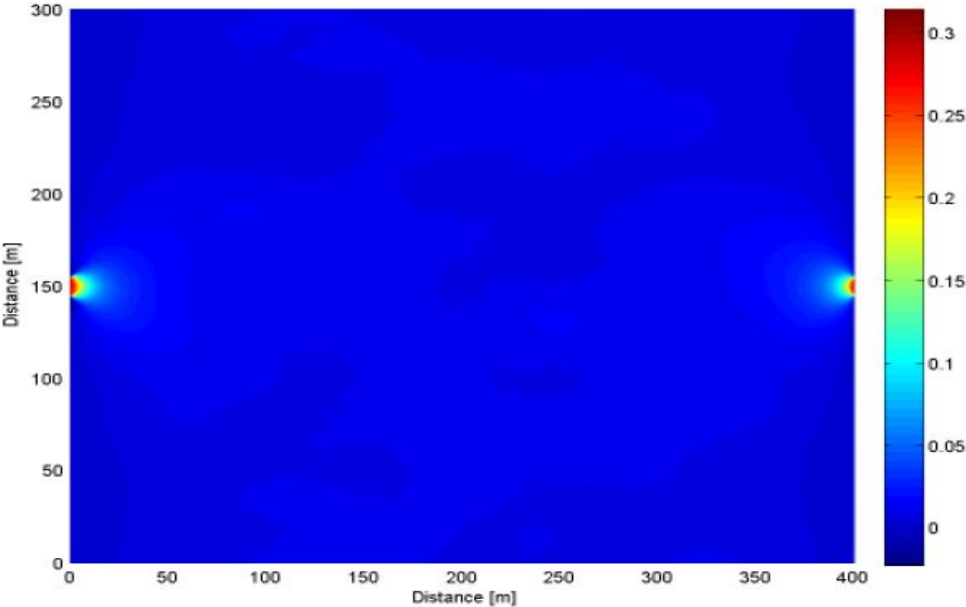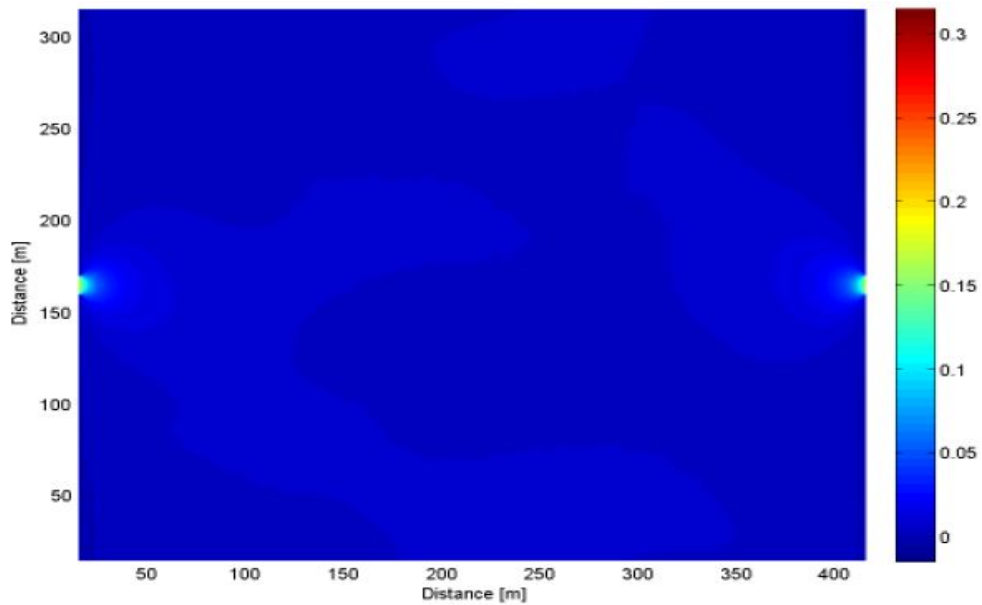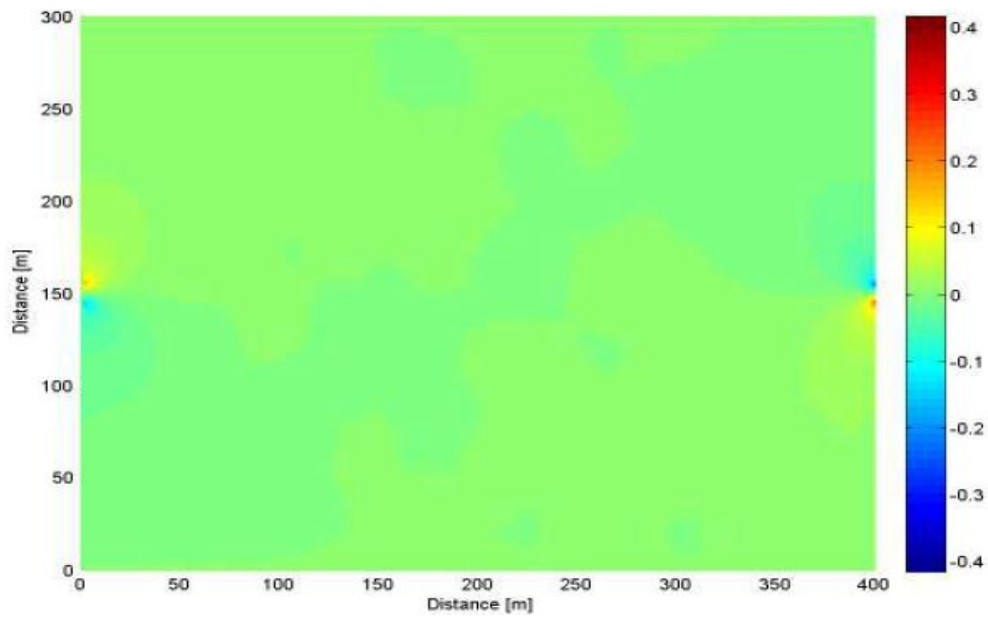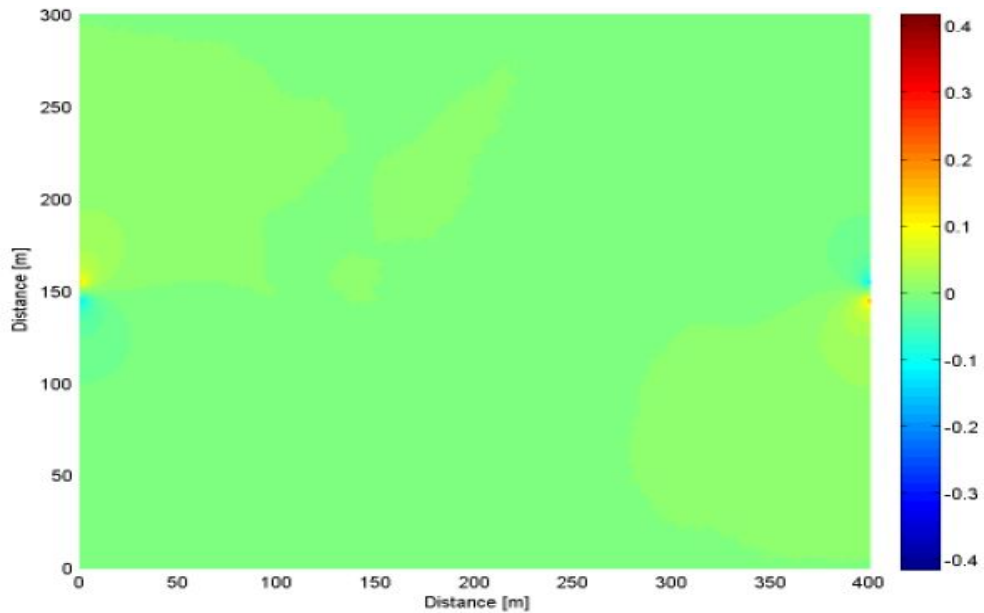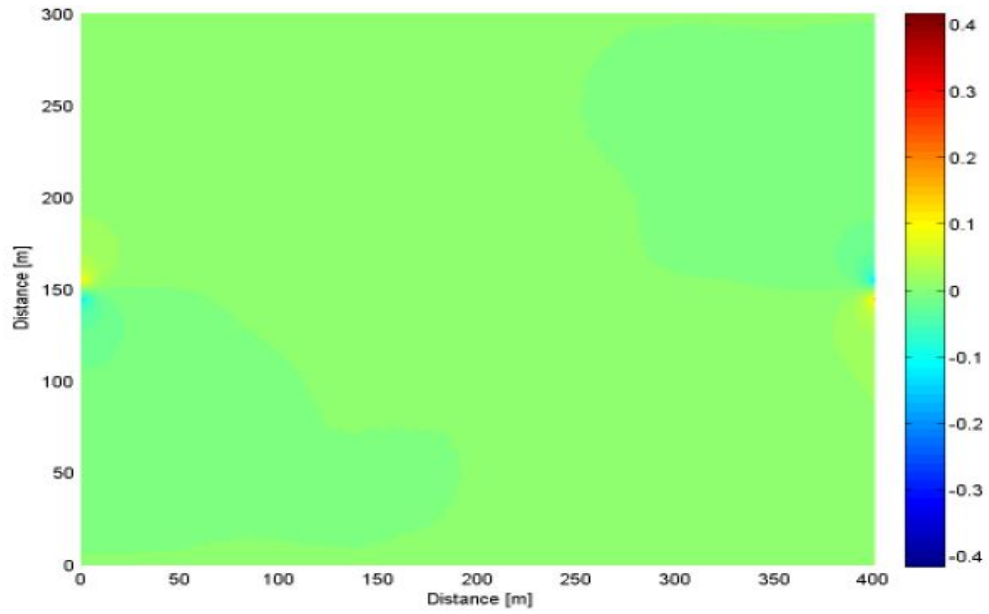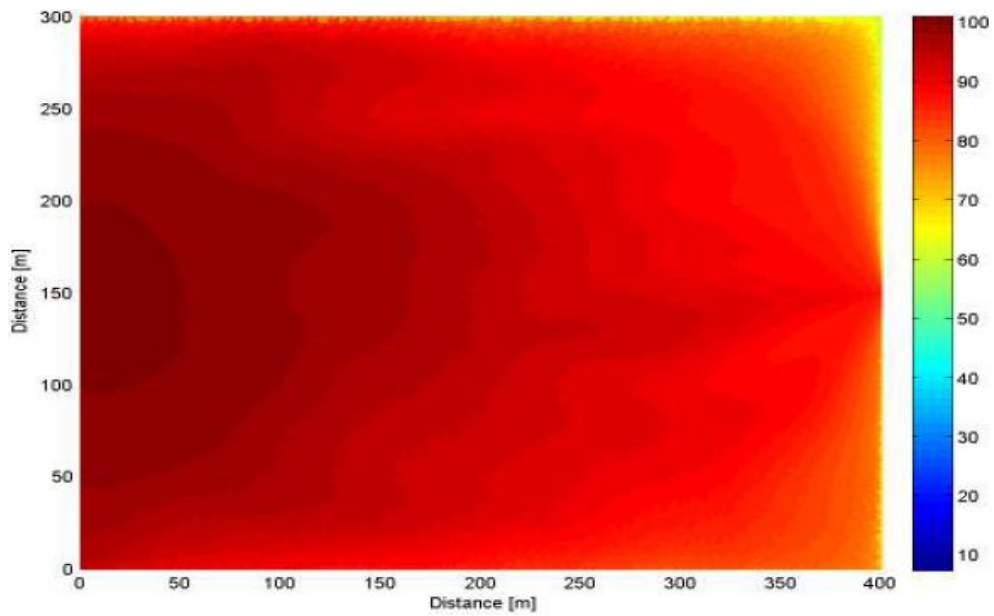

Figure 7.5. Velocity along x field for distributed vegetation field with the first statistics.
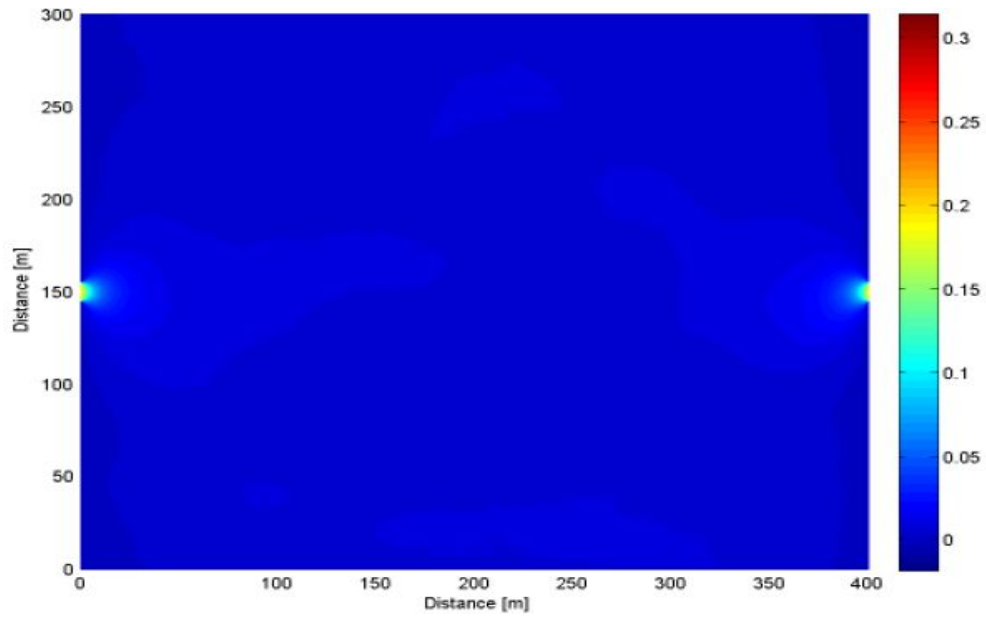
Figure 7.6. Velocity along x field for vegetation field with the second statistics.

Figure 7.7. Velocity along x field for distributed vegetation field with the third statistics.

- These pictures represent the distribution of the velocity along y-direction:

Figure 7.8. Velocity along y field for distributed vegetation field with the first statistics.

Figure 7.9. Velocity along y field for distributed vegetation field with thesecond statistics.

Figure 7.10. Velocity along y field for distributed vegetation field with the third statistics.

- These pictures represent the distribution of the pollutant concentration:

Figure 7.11. Concentration field for distributed vegetation field with the first statistics.
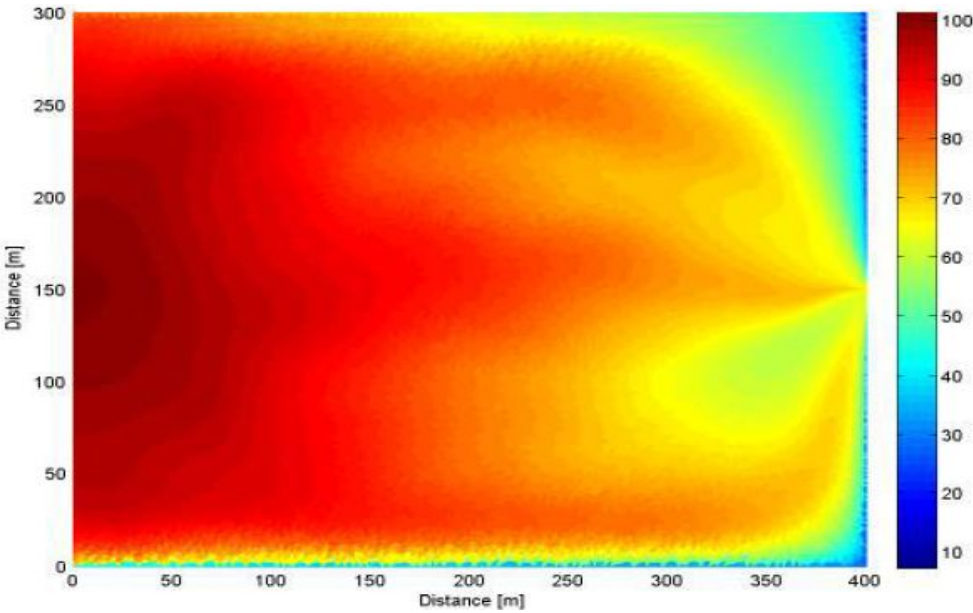
Figure 7.12. Concentration field for distributed vegetation field with thesecond statistics.
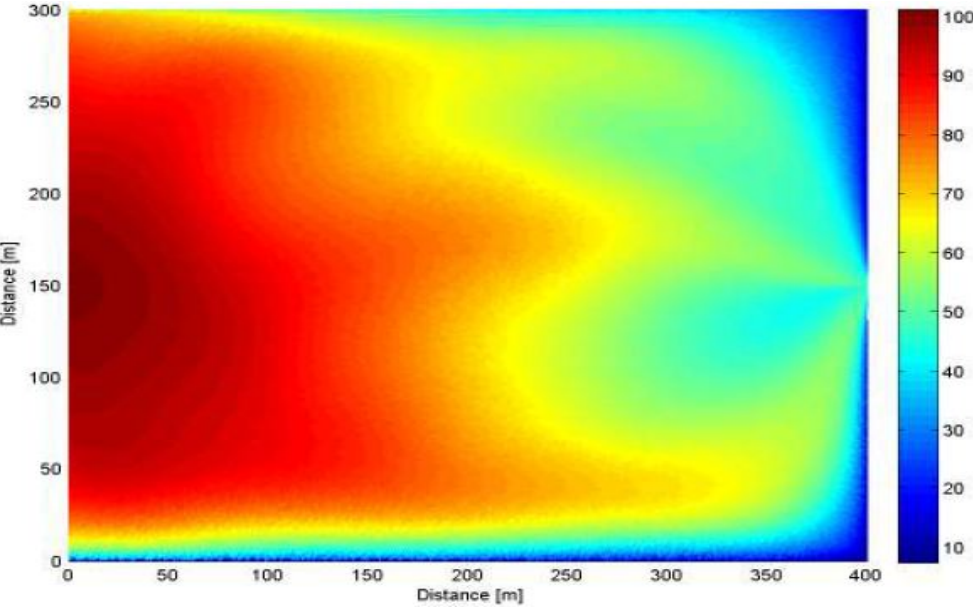

Figure 7.13. Concentration field for distributed vegetation field with the third statistics.

8

Results

In this chapter, a complete data analysis was conducted, using the collected data obtained from simulations. In particular, it has been tried to understand the relationship and the influence that the vegetation statistics have on the main wetland features: concentration efficiency, mass efficiency and flow rate.

Finally an attempt to assemble all the statistic variables and the concentration efficiency in two dimensionless parameters has been made.

8.1 Removal efficiency

The first two graphs show the behaviour of the discharge $Q[m^3/s]$ and the behaviour of the concentration removal efficiency, respect to the mean stem density. The concentration removal efficiency $E[-]$ is defined as:

$$E = \frac{C_{in} - C_{out}}{C_{in}} \tag{8.1}$$

where $C_{in} [mol/m^3]$ is the inlet concentration and $C_{out} [mol/m^3]$ is the outlet concentration.

As expected, it is possible to observe from the first graph (Figure 8.1) that the flow rate decreases (hence resident time increases) with the increase of the mean
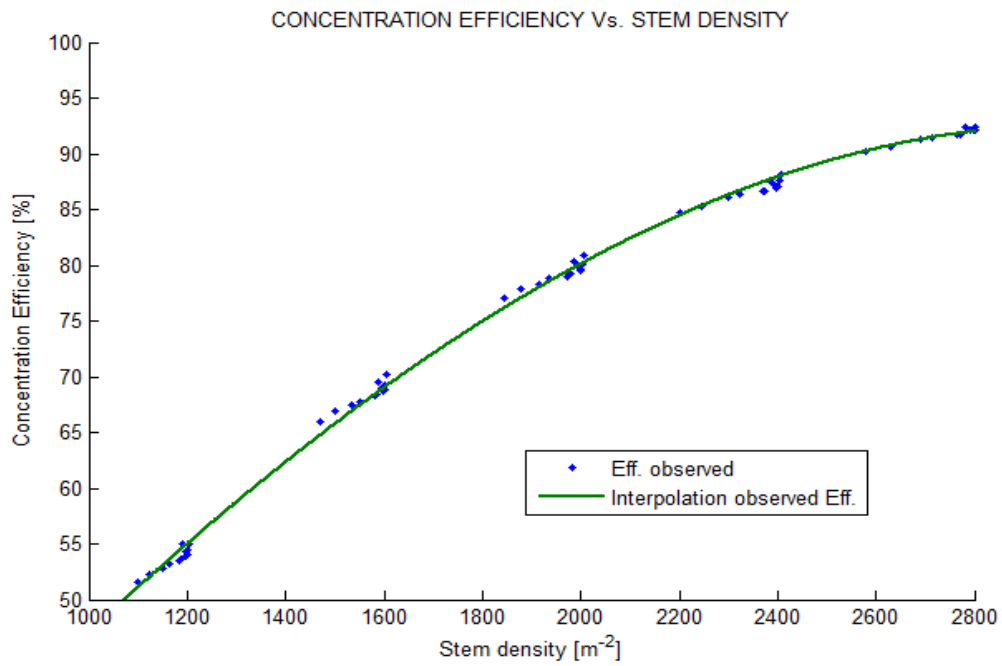
CONCENTRATION EFFICIENCY Vs. STEM DENSITY

Figure 8.1. Plot of concentration efficiency vs. mean stem density (field 120x90m).
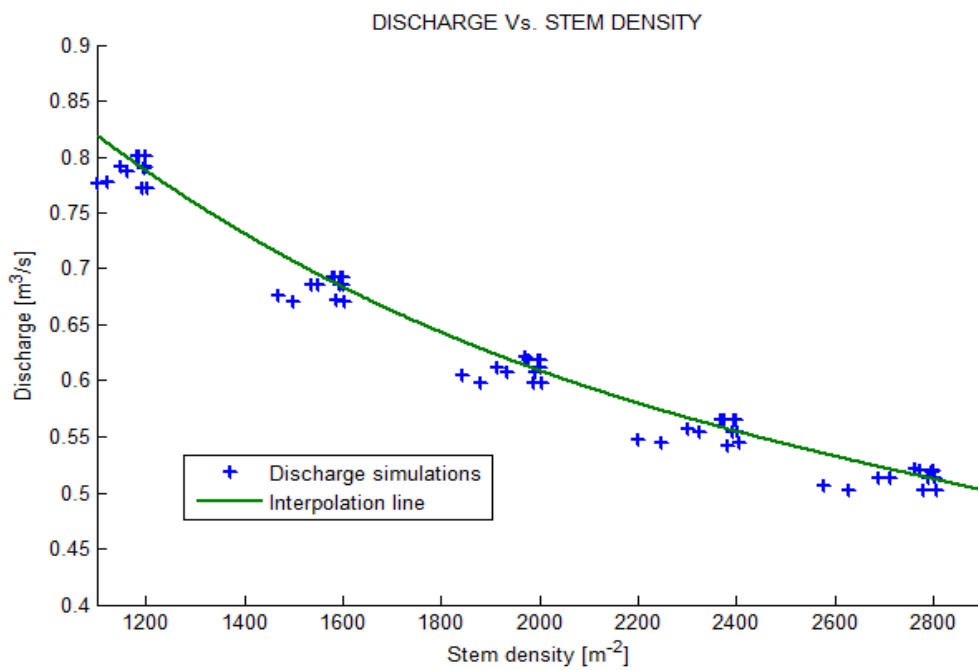
DISCHARGE Vs. STEM DENSITY

Figure 8.2. Plot of discharge vs. mean stem density (field 120x90m).

stem density, following a logarithmic profile. This is due to the proportional relationship between the shear stresses with the stem density.

The second graph (Figure 8.2) shows that for the concentration removal efficiency the most important statistics is the mean stem density, and that this efficiency increases with it, following a logarithmic profile too.

The superposition of these two graphs gives a third graph (Figure 8.3), which represents the mass efficiency against the mean stem density. The mass efficiency $E_m[mol/s]$ is defined as:

$$E_m = Q_{in}C_{in} - Q_{out}C_{out} \tag{8.2}$$
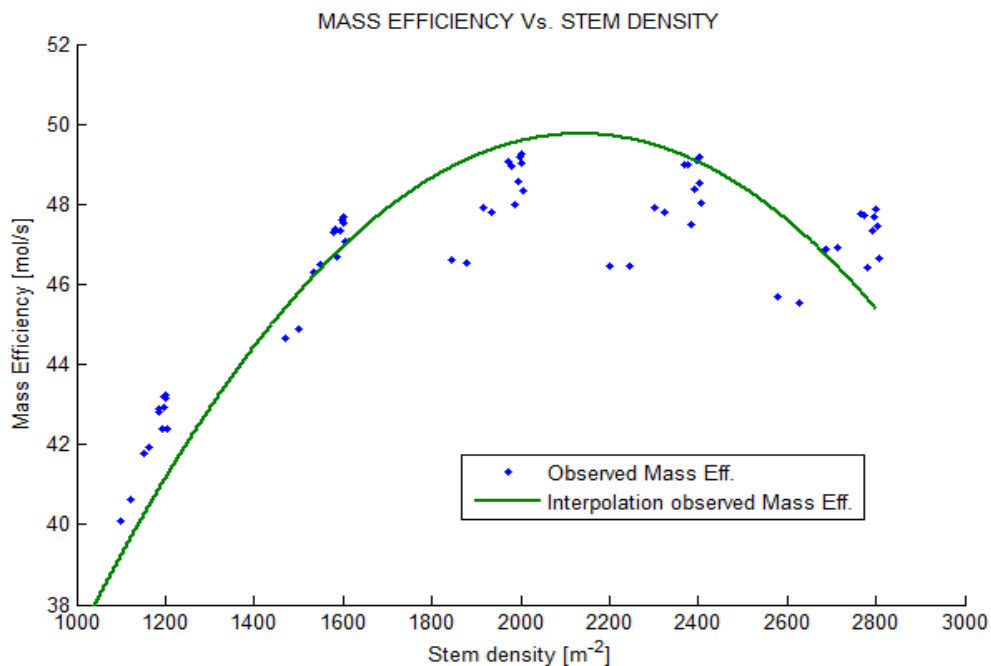
Figure 8.3. Plot of mass efficiency vs. mean stem density (field 120x90m).

Differently than for the previous graphs, which increase or decrease monotonically, this one can be subdivided in three parts:

- in the first part the curve growths; this happens because the increase of

concentration removal efficiency prevails on the discharge decrease;

- in the second part there is a maximum point, where the influence of the increse of the concentration removal efficiency is equal to the influence of the decrease of discharge;

- in the last part the curve decreases, because the increase of concentration efficiency can not compensate the discharge decrease.

From this plot is possible to see that mass removal efficiency is influenced also by the variance and the correlation length of the vegetation field. The following graph (Figure 8.4), where the lines interpolate points with same ratio μ/σ shows that for a fixed mean of stem density the mass removal efficiency decreases with the increase of the variance.
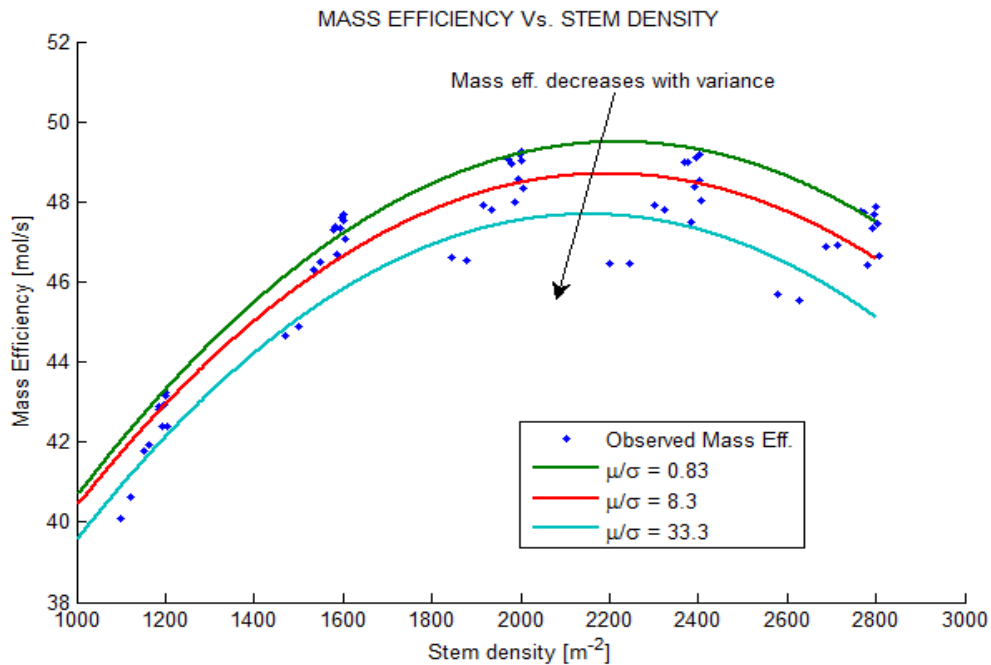
Figure 8.4. Plot of mass efficiency vs. mean stem density (field 120x90m).

Same thing happens for the increase of the correllation lenght (Figure 8.5)
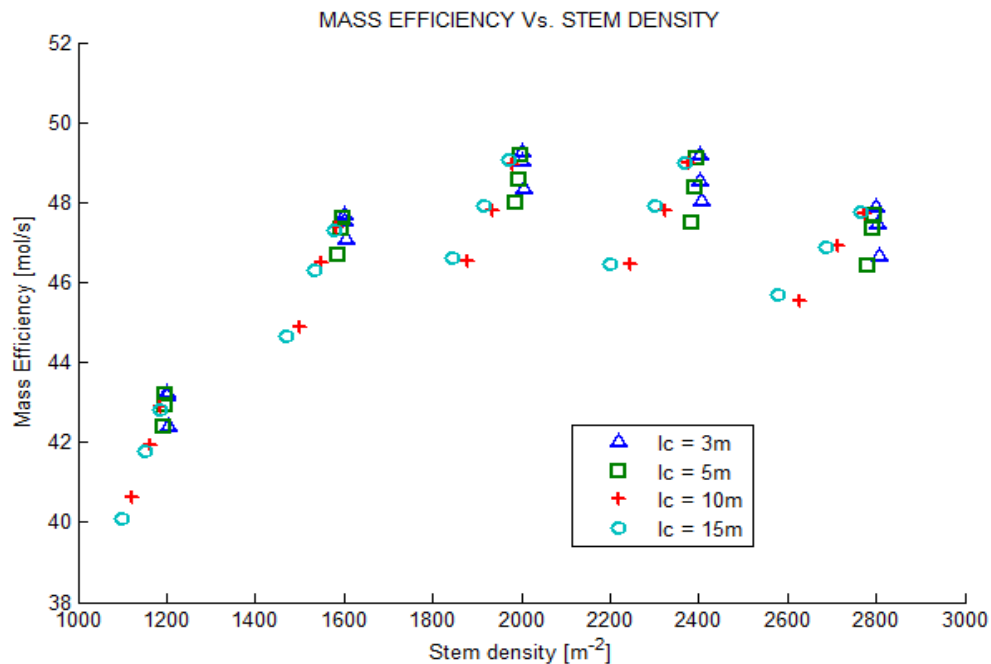
**Figure 8.5.** Plot of mass efficiency vs. mean stem density (field 120x90m).

In fact the increase af these two statistics lead to an increase of zones with very high vegetation density and zones with very low density of vegetation, favoring the formation of preferential patways, and then reducing the effective resident time of the system.

The next picture (Figure 8.6) shows a comparison between the curve given by the interpolation of the concentration efficiency, obtained through simulations, and the curve obtained considering the wetland as a CSTR system, with first order decay process.

It can be observed that the first curve lays under the second one, and only for efficiency around 1 they tend to converge. The reason of this behaviour, should be probabily due to the fact that when the wetland is assumed as a CSTR system, all its volume is assumed to be effective for the resident time, while because the model considers the formation af preferential pathways, caused by vegetation distribution, its effective volume results to be reduced and then the resident time

too.

Hence for this second case, the concentration efficiency, being proportional to the resident time, will be lower.
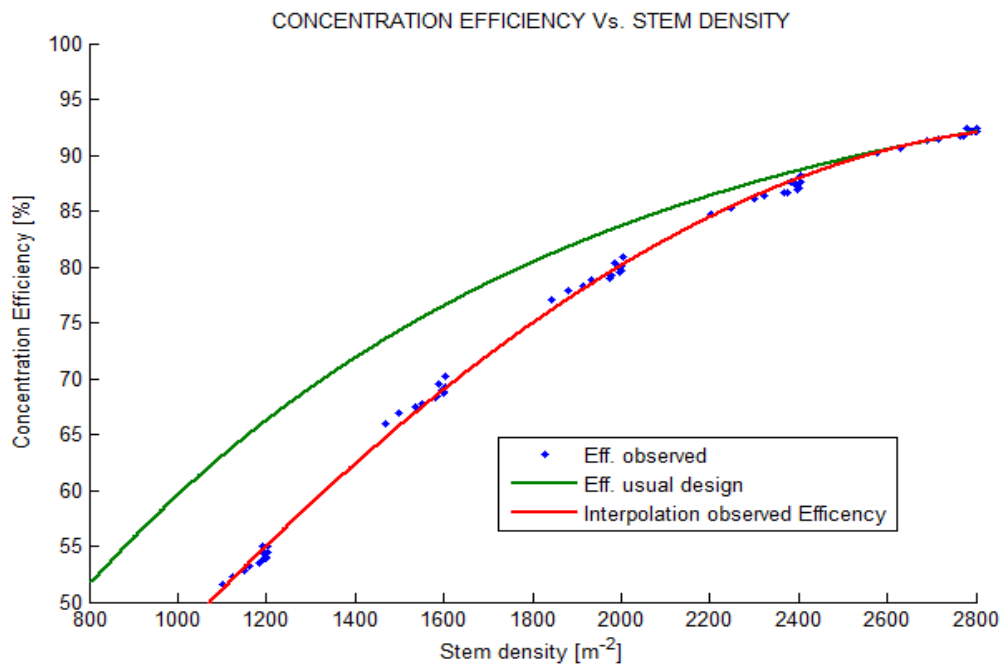
Figure 8.6. Comparison between concentration efficiency by simulations and by considering a CSTR system (field 120x90m).

8.2   Dimensional analysis

Here it is tried to find two dimensionless parameters in order to correlate all the statistics with the concentration removal efficiency. For doing this, they have been considered two further variables M_x and M_y $[m]$:

$$M_x = \sum_i |\, \mu_i \, A_i \, y_i|; \qquad M_y = \sum_i |\, \mu_i \, A_i \, x_i|; \qquad (8.3)$$

where $\mu_i [m^{-2}]$ is the density of steams, for the area $A_i [m^2]$, while $x_i [m]$ and $y_i [m]$ are the distances between the simmetrical axes. These varables are used because, fields with same statistics (mean, variance and correlation length) are not unically definied and because the stem concentration can have different impact depending on where it is situated respect to the flow.
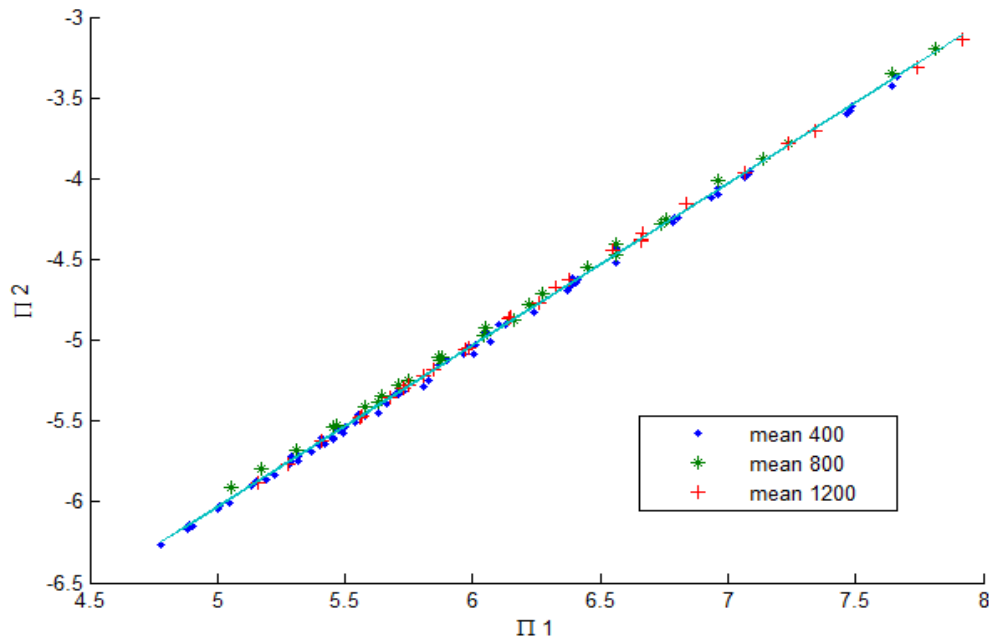

Figure 8.7. Plot of two dimensionless variables (field 400x300m).

85

The dimensionless parameters $\Pi 1$ and $\Pi 2$ are defined as:

$$\Pi 1 = log(\frac{(M_x + M_y)^{1/2} \, \sigma^{1/2}}{l_c \, \mu^{4/3}}); \quad \Pi 2 = log(\frac{E_c^{3/2} \, \sigma^{1/2}}{l_c \, \mu})$$ (8.4)

where σ^2 is the variance and l_c the correlation length of the vegetation field.

As it possible to see from the graph above (Figure 8.7), the dimensionless paramiters $\Pi 1$ and $\Pi 2$ are linearly proportional. Their relationship is:

$$\Pi 2 = 1.01 \, \Pi 1 - 11.04$$ (8.5)

Chapter 9

Summary and conclusion

The objective of this thesis can be summarised in identifying the influence of vegetation statistics on the wetland concentration and mass efficiencies.

The main findings are shown as follows:

- the concentration efficiencies obtained by simulations are always lower than the concentration efficiencies obtained considering the wetland as a CSTR system, because the formation of preferential pathways which lead to a decrease of the residential time. They tend to converge when the efficiency is near to one.

- the most influent parameter for both concentration and mass efficiencies is the mean steam density which influence both the hydraulics and the decay rate of the model;

- increasing the mean density of vegetation, concentration removal efficiency monotonically increases, while the discharge monotonically decreases, both with a logarithmic profile;

- the mass efficiency, obtained by the composition of concentration efficiency and discharge, has a point of maximum;

- increasing the variance and correlation length, the mass efficiency decreases because they favor the formation of preferential pathwas;

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