



A Modeling Framework for Hyporheic Flow within Hydrodynamics Scale

Antonio Preziosi-Ribero

Universidad Nacional de Colombia
Facultad de Ingeniería, Área Curricular de Ingeniería Civil y Agrícola
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Antonio Preziosi-Ribero

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Advisor:

Leonardo David Donado, PhD
Professor, Universidad Nacional de Colombia

Co-Advisor:

Jorge A. Escobar-Vargas, PhD
Associate Professor, Pontificia Universidad Javeriana

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In memoriam: HK3-EPV

“He who does not respect his own conscience will never be respected by others”

A.L. Cauchy

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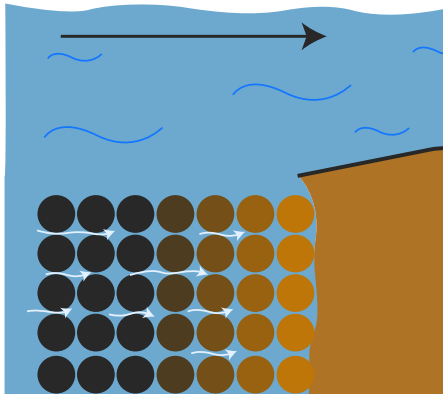
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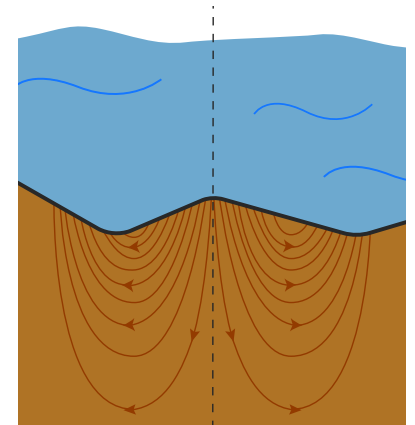
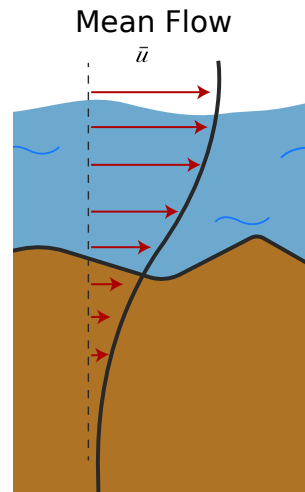
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Graphical Abstract



Detailed Flow

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nu \Delta \mathbf{u}$$



Particle Tracking

$$x(t + \Delta t) = x(t) + u_x \Delta t + \xi \sqrt{2D_x \Delta t}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla P + \nu \Delta \mathbf{u} + \epsilon \mathbf{u} + \beta \mathbf{u} \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = 0$$

Resumen

En países tropicales como Colombia y en gran parte del mundo, las corrientes superficiales juegan un rol importante como fuente de agua potable para grandes asentamientos humanos, a la vez que receptores de vertimientos domésticos e industriales. El crecimiento de la población, la migración interna a las ciudades y los efectos del cambio climático, hacen que la presión sobre los ecosistemas acuáticos se vuelva un tema de interés para la ciencia y la administración pública. En consecuencia, el entendimiento de los diferentes cuerpos de agua, las relaciones entre ellos y su modelación integral son un tema de investigación con gran acogida en las geociencias y la ingeniería. De hecho, desde hace cerca de 30 años, la academia se ha fijado en las realciones entre las corrientes de agua y los acuíferos debajo de las mismas para estudiar diferentes fenómenos ocasionados por este tipo de flujos. De esta forma nace el estudio del Flujo Hiporreico (HF) y la Zona Hiporreica (HZ).

La Zona Hiporreica (HZ) se define como “la trayectoria de flujo de agua que ha abandonado un cuerpo de agua superficial hace “poco” tiempo, para mezclarse con agua subterránea y “pronto” volver al mismo cuerpo de agua”. Este lugar tiene gran importancia en procesos ecológicos, biológicos y químicos como la atenuación de contaminantes, el transporte de nutrientes, sedimentos y calor para el crecimiento de biota, los procesos de nitrificación de los cuerpos de agua y la restauración de cuerpos de agua. Estos fenómenos están ligados estrechamente con el concepto de calidad y química del agua, y son modelados con ecuaciones de transporte conservativo o reactivo. No obstante, el transporte de sustancias en este medio depende del flujo de agua y los patrones que este sigue.

Al flujo de agua en la HZ se le denomina Flujo Hiporreico (HF), y su principal característica es el amplio rango de escalas en el que está presente. De esta forma, dentro de la HZ se pueden observar flujo desde la escala de poros, controlado por gradientes de presión, hasta la escala de flujos controlados por la morfología de las corrientes de agua. Esta amplia variedad de escalas, sumada a la heterogeneidad de los medios naturales, hacen que el estudio de procesos en la HZ se transforme en un reto para la comunidad científica.

El objetivo del presente trabajo de investigación es el de formular un marco metodológico para la modelación de la HZ desde la perspectiva de la mecánica del medio continuo. Para tal fin, este trabajo presenta un estudio del HF, a partir de diferentes modelos numéricos, proponiendo simplificaciones que puedan representar el HF. Asimismo, el uso de modelos numéricos permite descomponer los fenómenos físicos para caracterizar la contribución de cada uno al HF. Los resultados de los modelos son comparados con resultados experimentales para verificar su utilidad práctica y proponer su uso en diferentes casos de estudio relacionados con procesos biológicos, químicos y ecológicos.

Para el cumplimiento del objetivo general se presentan tres aproximaciones de modelación de Flujo Hiporreico dominado por factores hidrodinámicos, por medio de diferentes herramientas numéricas. Estas aproximaciones se basan en la mecánica del medio continuo, a pesar de utilizar diferentes esquemas numéricos; presentan diferentes fortalezas y debilidades y, sobre todo, brindan información sobre el Flujo Hiporreico que, en un futuro, puede ser escalada

para contribuir con la toma de decisiones en lo referente al recurso hídrico.

El primer modelo numérico propuesto utiliza la ecuación de Burgers (BE) para representar el HF en un lecho de esferas dispuestas en forma cúbica. El objetivo principal es estudiar el decaimiento de las velocidades turbulentas dentro de un medio uniforme para caracterizar el HF mediante una expresión simple como la BE teniendo en cuenta la interacción de efectos no lineales y disipación de energía, propios de los flujos multiescala. Para el modelo computacional se utilizó un método de multidominio espectral (SMPM) para evitar errores numéricos asociados a los métodos tradicionales como las diferencias, elementos o volúmenes finitos. Este modelo se presenta como una primera aproximación hacia el HF a escala de laboratorio.

En segundo lugar, se propone un modelo basado en las ecuaciones de Navier-Stokes (NSE) modificada para representar la combinación de un flujo libre y el lecho de un canal. De nuevo, el objetivo es determinar un perfil de velocidades promedio que represente la transición entre el flujo de un canal y un lecho de forma regular. Para este fin se utilizó el método de los volúmenes finitos y un paquete de software de código abierto que fue modificado para incluir viscosidades diferentes y términos de fuente/sumidero que representen el decaimiento de velocidades. Los resultados de flujo son comparados con diferentes modelos numéricos y experimentales. De igual manera, este análisis incluye además una implementación de transporte conservativo de especies que fue también comparado con resultados experimentales.

Como última aproximación, se propone un modelo de rastreo numérico de partículas para evaluar la influencia del HF en la depositación de sedimentos finos en lechos de ríos. El objetivo principal de este aparte es analizar el proceso de depositación de sedimentos, teniendo en cuenta diferentes escenarios de flujo en la HZ. Además del flujo en el medio poroso, el modelo implementado utiliza la filtración de materiales dentro del lecho para retener partículas finas y mostrar los lugares donde se espera que haya mayor depositación de estas. Los resultados, una vez más, son validados de forma cualitativa con experimentos de laboratorio realizados con kaolinita en canales recirculantes experimentales.

En síntesis, los tres modelos presentados en este trabajo ofrecen una visión novedosa sobre el Flujo Hiporreico en escalas dominadas por efectos hidrodinámicos. Principalmente, el dominio de las condiciones de flujo libre presentes sobre el flujo en el medio poroso y la presencia de flujos con altos números de Reynolds dentro del medio poroso dominan la hidrodinámica y los procesos asociados a la misma, como la despositación de sedimentos finos.

Abstract

In tropical countries, like Colombia and in other parts of the world, free surface streams play a key role either as freshwater supply for human settlements, or as wastewater receivers from households and industrial compounds. Population growth, internal migration of people towards cities and the effects of climate change make that pressure on aquatic ecosystems become a topic of interest for science and public administration. Therefore, understanding different water bodies, their interaction and their integral modelling process are a research topic of great interest in earth sciences and engineering. In fact, in the last 30 years, academia has studied the interaction between free surface streams and aquifers beneath them, focusing on the effects of these type of flows. This milestone marked the beginning of the studies of Hyporheic Flow (HF) and Hyporheic Zone (HZ).

Hyporheic Zone (HZ) is defined as “a subsurface flowpath along which water ‘recently’ from the stream will mix with subsurface water to ‘soon’ return to the stream”. This place has a great relevance in ecologic, biologic and chemical processes such as contaminant attenuation, nutrient, sediment and heat transport for biota growth, nitrification processes in water bodies and river restoration. These phenomena are closely related with chemical water quality and are modeled usually with conservative and reactive transport equations. Nevertheless, species transport in HZ depends on water flow and the patterns it follows.

The flow within the HZ is known as Hyporheic Flow (HF) and its main feature is the wide range of scales in which it acts. Hence, within HZ there is flow from the pore scale and it is controlled by pressure gradients, to the scale of flows controlled by the stream morphology. This wide variety of scales, along with media heterogeneity make the study of processes within the HZ a challenge for the scientific community. Moreover, in countries like Colombia, streams play a key role in society since they are the main freshwater supply and also receive the water disposal.

The main goal of this research project is to formulate a methodological frame for HZ modelling from the continuous media perspective. To that end, this work presents the study of HF, starting from different numerical models, proposing simplifications that can portray HF. In the same way, the use of numerical models allows the decomposition of the physical phenomena to characterize their individual contribution to the HF. The models’ results are compared with experimental results to validate their practical usefulness and propose their use in different case studies related with biological, chemical and ecological processes.

To accomplish the main goal, this document presents three different approaches to HF driven by hydrodynamics, using different numerical tools. These approaches are based in continuum media mechanics, despite using different numerical schemes; each one of the presents pros and cons, but above all, each one of them gives key information about Hyporheic Flow that, in the near future, can be upscaled and used for decision making regarding hydraulic resources.

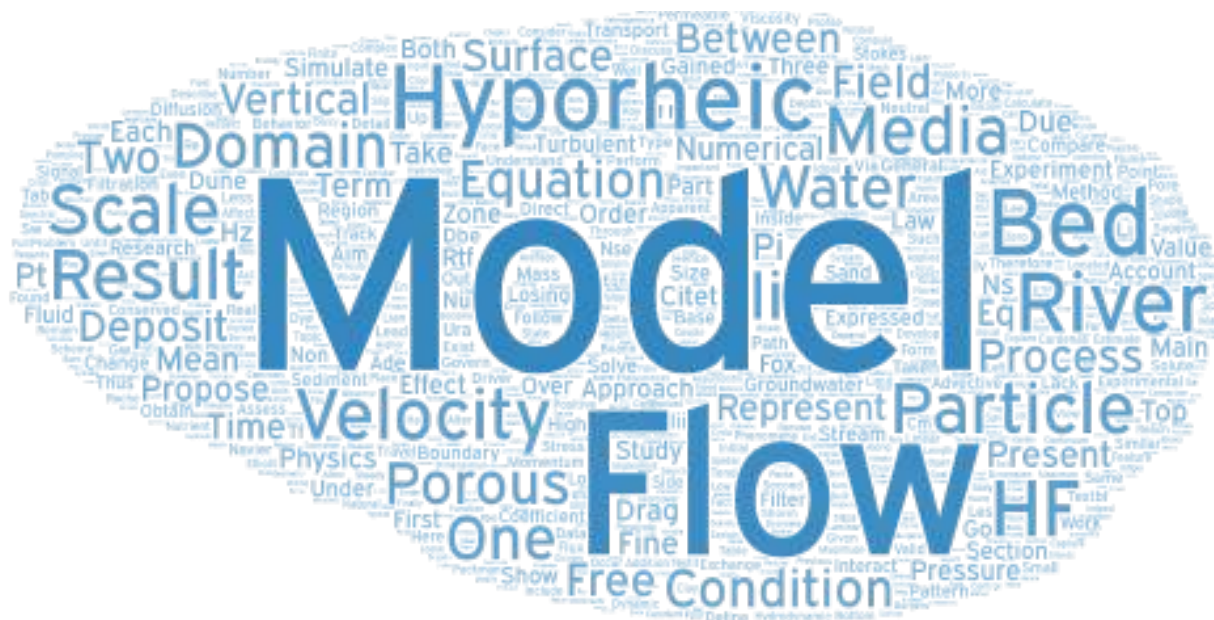
The first numerical model proposed uses Burgers’ Equation (BE) to represent HF in a bed with cubical packed spheres. The main goal is to study turbulent velocity decay within uni-

form media to characterize HF through a simple expression as the BE taking into account the interaction between non linear effects and energy dissipation, characteristic within multiscale flows. For the computational model a Spectral Multidomain Penalty method (SMPM) to avoid numerical errors associated with traditional numerical schemes as finite differences, elements or volumes. The BE model is presented as a first approach of HF in a lab scale.

In second place, the use of the Navier-Stokes Equations (NSE) to represent the combination of free surface flow and a sand bed. Again, the main goal is to determine a mean velocity profile representing the transition between free surface flow in a flume and a regular bed. To achieve this goal the Finite Volume Method was used along with an open source code that was modified to include different viscosity values and source/sink terms that are able to capture the velocity decay. The results of flow are compared with different numerical and experimental models. This analysis includes also a conservative transport model that was also compared with experimental results.

For the final approach, a numerical particle-tracking model is proposed to assess the influence of HF in fine sediment deposition in river beds. The main goal of this part is to evaluate the process of deposition taking into account different flow scenarios within the HZ. Besides flow in porous media, this model includes particle filtration within the bed to retain particles and show places where deposition is more prone to occur. The results, once again, are compared with flume experiments of kaolinite deposition in a recirculating flume.

To wrap up, the three models presented in this work offer a novel vision on Hyporheic Flow within scales driven by hydrodynamical effects. Mainly, the free flow conditions driving flow in porous media and high Reynolds number flows presence within porous media determine hydrodynamics and processes associated with it, such as fine sediment deposition.



Keywords

Keywords: Hyporheic Flow, Model, Groundwater-Surface Water Processes, Fluid Mechanics, River Bed

Palabras clave: Flujo Hiporreico, Modelo, Procesos Agua Superficial - Agua Subterránea, Mecánica de Fluidos, Lechos de río

Related Publications

Peer-reviewed articles

Antonio Preziosi-Ribero, Aaron I. Packman, Jorge A. Escobar-Vargas, Colin B. Phillips, Leonardo David Donado, Shai Arnon (2020). Fine Sediment Deposition and Filtration Under Losing and Gaining Flow Conditions: A Particle Tracking Model Approach. *Water Resources Research*. February 2020. DOI: 10.1029/2019WR026057

Antonio Preziosi-Ribero, Edwin Saavedra-Cifuentes, Jorge A. Escobar-Vargas, Leonardo David Donado (2017). A High Order Element Based Method to Estimate Hyporheic Flow in Rivers Using the Burgers' Equation. Proceedings of the 37th IAHR World Congress. SSN 1562-6865 (Online) - ISSN 1063-7710 (Print)

Edwin Y. Saavedra-Cifuentes, **Antonio Preziosi-Ribero**, Jorge A. Escobar-Vargas, Leonardo David Donado (2020). Hydrodynamics coupling of a free surface flow over a permeable porous bed. *In preparation For Water resources Research*

Oral presentations

Antonio Preziosi-Ribero, Jorge Peñaloza-Giraldo, Jorge Escobar-Vargas, Leonardo David Donado (2016). A High Order Element Based Method for the Simulation of Velocity Damping in the Hyporheic Zone of a High Mountain River. Geophysical Research Abstracts. EGU General Assembly 2016

Edwin Y. Saavedra-Cifuentes, **Antonio Preziosi-Ribero**, Jorge A. Escobar-Vargas, Leonardo David Donado (2017). Impact of Boundary Conditions on a Numerical Model of Flow Over a Porous Bed as an Approach of a River's Hyporheic Zone. E-proceedings of the 37th IAHR World Congress. Kuala-Lumpur, Malaysia.

Antonio Preziosi-Ribero, Edwin Y. Saavedra-Cifuentes, Jorge A. Escobar-Vargas, Leonardo David Donado (2017). A High Order Element Based Method to Estimate Hyporheic Flow in Rivers Using the Burgers' Equation. E-proceedings of the 37th IAHR World Congress. Kuala-Lumpur, Malaysia.

Antonio Preziosi-Ribero, Jorge A. Escobar-Vargas, Aaron I. Packman, Edwin Y. Saavedra-Cifuentes, Leonardo David Donado (2017). A Numerical Approach to Hyporheic Flow and Velocity Damping in a Two Dimensional Ideal Porous Media. ICGW 2017. Bogotá,

Colombia

Antonio Preziosi-Ribero, Aaron I. Packman, Aryeh Fox, Jorge A. Escobar-Vargas, Leonardo David Donado, Angang Li, Shai Arnon (2017). A Particle Tracking Model for Suspended Sediment Transport and Streambed Clogging under Losing and Gaining Conditions. AGU Fall Meeting 2017

Antonio Preziosi-Ribero, Aaron I. Packman, Jorge A. Escobar-Vargas, Leonardo David Donado (2018). A Particle-Tracking Model to Estimate Clay Deposition in an Experimental Flume Under Losing-Gaining Flow Conditions. AGU Fall Meeting 2018.

Antonio Preziosi-Ribero, Jorge A. Escobar-Vargas, Sergio A. Castiblanco-Ballesteros, Leonardo David Donado (2019). A Numerical Model to Simulate Turbulent Velocity Decay within Porous Beds Using Surface Velocity and the Burgers Equation. AGU Fall Meeting 2019

Codes/Repositories

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Antonio Preziosi-Ribero, Jorge A. Escobar-Vargas, Sergio A. Castiblanco-Ballesteros, Leonardo David Donado (2017). 2D Burgers Equation Solution via SMPM with Continuous Boundary Condition (V0.1). <http://www.github.com/apreziosir/2DBurgers>

Table of Contents

Acknowledgements	VII
Resumen-Abstract	x
Related Publications	xv
Symbols with Latin Letters	xix
Symbols with Greek Letters	xx
Acronyms	xxi
List of Tables	xxi
List of Figures	xxii
1 Introduction	1
2 General Outline	5
2.1 Domains/Scales within River Corridor	6
2.1.1 Hydrogeological Scale - Geological and Lithotopo Processes Domain .	8
2.1.2 Hydrological Scale - Reach Domain	8
2.1.3 Hydrodynamics or Ecological Scale - Feature and Grain Processes Do- mains	8
2.2 Fluid Dynamics and Hyporheic Flow	12
2.3 HF Models: State of the Art	15
2.3.1 Coupling of Navier-Stokes and Darcy Law	15
2.3.2 Velocity Damping Models	17
2.3.3 Oceanography Example	20
2.3.4 Numerical Particle-Tracking	21
2.4 Numerical Tools	22
2.5 Summary	23
3 A Simple Hydrodynamics Profile for Hyporheic Flow	24
3.1 Introduction	24
3.2 Conceptual and Mathematical Model	25
3.2.1 Conceptual Model	25
3.2.2 Numerical Model	27

3.3	Results and Discussion	29
3.4	Conclusions	34
4	Coupling Free Surface Flow over Permeable Porous Beds	37
4.1	Introduction	38
4.2	Proposed Model	40
4.3	Benchmark Case Comparison	41
4.4	Laboratory Experiment and Validation	43
4.4.1	Computational Domain	44
4.4.2	Velocity Fields and Free Surface Flow behaviour	44
4.4.3	Scalar Transport Simulation	46
4.5	Discussion	47
4.6	Conclusions	49
5	Combining Hyporheic Hydrodynamics and Fine Sediment Deposition	51
5.1	Introduction	52
5.2	Methods	54
5.2.1	Conceptual model	54
5.2.2	Mathematical Model	56
5.2.3	Numerical Model	60
5.3	Results	61
5.4	Discussion	67
5.5	Conclusions	70
6	Discussion, Conclusions and Outlook	71
6.1	Discussion	71
6.2	Conclusions	73
6.3	Outlook	74
	References	76

Symbols with Latin letters

Symbol	Term	Dimensions
A	Area	L^2
C	Concentration	ML^{-3}
D	Diffusion Coefficient	L^2T^{-1}
f	External Forces	MLT^{-2}
g	Gravity Constant	LT^{-2}
h	Hydraulic Head	L
H	Mean Water Height	L
k	Permeability	L^2
K	Hydraulic Conductivity	LT^{-1}
m	Mass	M
P	Pressure	$ML^{-1}T^{-2}$
$\mathcal{P}$	Stress Tensor	$ML^{-1}T^{-2}$
p_{ii}	Normal Stress Component	$ML^{-1}T^{-2}$
p_{ij}	Shear Stress Component	$ML^{-1}T^{-2}$
q	Darcy Velocity	LT^{-1}
Q	Flow rate	L^3T^{-1}
t	Time	T
$\mathcal{T}$	Deviatoric Stress Tensor	$ML^{-1}T^{-2}$
u	Flow Velocity	LT^{-1}
V	Volume	L^3
w	Advection Velocity	L^2T^{-1}
W	Weight	MLT^{-2}

Symbols with Greek Letters

Symbol	Term	Dimensions
α	TSM Exchange coefficient	—
γ	Specific Weight	$ML^{-2}T^{-2}$
Γ	Memory Function	<i>Function</i>
ϵ	Rate of Strain Tensor	—
ϵ_{ii}	Axial Component Rate of Strain Tensor	—
ϵ_{ij}	Tangential Component Rate of Strain Tensor	—
η	Free Surface Water Position	L
κ	Effective Thermal Conductivity	$MLT^{-3}\theta^{-1}$
μ	Dynamic Viscosity	$ML^{-1}T^{-1}$
ν	Kinematic Viscosity	L^2T^{-1}
ν_t	Turbulent Viscosity	L^2T^{-1}
ν_a	Apparent Viscosity	L^2T^{-1}
ρ	Density	ML^{-3}
σ	Stress tensor axial component	$ML^{-1}T^{-2}$
σ'	Electric Conductivity	$M^{-1}L^{-2}T^3I^2$
τ	Stress tensor tangential component	$ML^{-1}T^{-2}$
— <i>Dimensionless</i>		

Acronyms

Abbrviation	Term
<i>ADE</i>	Advection Diffusion Equation
<i>APM</i>	Advective Pumping Model
<i>BTC</i>	Break-Through Curve
<i>CFD</i>	Computational Fluid Dynamics
<i>CFL</i>	Courant-Friedrichs-Lewy Stability Criterion
<i>EC</i>	Electric Conductivity
<i>DG</i>	Discontinuous Galerkin Method
<i>FDM</i>	Finite Differences Method
<i>FEM</i>	Finite Elements Method
<i>FVM</i>	Finite Volume Method
<i>GW</i>	Groundwater
<i>HF</i>	Hyporheic Flow
<i>HZ</i>	Hyporheic Zone
<i>MRMT</i>	Multi-Rate Mass Transfer
<i>NSE</i>	Navier-Stokes Equations
<i>RCE</i>	River-Corridor Exchange
<i>RBf</i>	River-Bank Filtration
<i>RTD</i>	Residence Time Distribution
<i>SMPM</i>	Spectral Multi-Domain Penalty Method
<i>SW</i>	Surface Water
<i>TSM</i>	Transient Storage Model

List of Tables

2-1	Mass and Momentum Conservation Laws in Fluid Dynamics	13
2-2	Basic Flow Equations for the research project	13
2-3	Generic properties of most widely used numerical methods	23
5-1	Physical parameters (Packman et al., 2000b; Fox et al., 2014, 2018) for the comparison of the implemented Particle-Tracking model.	56

List of Figures

2-1	Cross section and Plan view of different scales of GW-SW interactions. From: Barthel and Banzhaf (2015).	7
2-2	Conceptual model of Hydrogeological scale. From: Buss et al. (2009)	9
2-3	Conceptual model of Hydrological scale. From: Buss et al. (2009)	10
2-4	Conceptual model of biogeochemical scale. From: Buss et al. (2009)	11
2-5	Conceptual model of Vaux proposition for HF. From: Tonina and Buffington (2009)	14
2-6	Spatial and temporal timescales for SW-GW interaction. Adapted from Boano et al. (2014)	15
2-7	Conceptual domain adapted from: Discacciati et al. (2002)	16
2-8	Discacciati et al. Coupling model. Adapted from: Discacciati et al. (2002) . .	17
2-9	Cardenas and Wilson conceptual 2D model. Adapted from: Cardenas and Wilson (2007c)	18
2-10	Velocity pulse modeled by Higashino and Stefan and Peñaloza-Giraldo et al. Adapted from: Higashino and Stefan (2008)	19
2-11	Conceptual Model for velocity damping. Adapted from: Peñaloza-Giraldo et al. (2015)	20
2-12	Conceptual Model in oceanography. From: Huang et al. (2008)	21
2-13	Error of collocation method against high order finite difference method. From: Canuto et al. (2009)	22
3-1	Conceptual model of velocity attenuation within an idealized porous media. The velocity over a vertical profile is expected to decay in magnitude and to have a decay in RMS. In this figure x and u stand for streamwise coordinate and velocity and z and w stand for vertical coordinate and velocity, respectively. The conceptual model is an adaptation from Lian et al. (2019).	26
3-2	Node location for the problem (brown points). Note that the domain only corresponds to the river bed and does not include the free surface flow and that the coordinate $(x, z = 0)$ correspond to the separation between the stream and the bed. The computational domain is composed by 30 subdomains in the streamwise direction and 15 subdomains in the vertical direction. Subdomains have five points within them.	29
3-3	Streamwise velocity signals extracted at different depths at equal times. In blue: the input signal gathered from the LES model. In orange, green, red and purple: signals generated by the 2DBE model.	30

3-4	Vertical velocity signal extracted at different depths at equal times. In blue: the input signal gathered from the LES model. In orange, green, red and purple: signals generated by the 2DBE model.	30
3-5	Normalized mean profiles: A. Streamwise velocity. B. Vertical velocity. For both of the plots, continuous lines indicate results from 2DBE.	32
3-6	Normalized mean stresses profiles: A. streamwise turbulent stress, B. vertical turbulent stress and C. Reynolds stress. For all of the plots, continuous line indicate results from 2DBE.	32
3-7	Mean nondimensional velocity heatmaps. A. Streamwise velocity. B. Vertical velocity. Domain is normalized by the mean particle diameter from the LES model (Lian et al., 2019).	33
3-8	Mean turbulent stresses over the entire domain. Stresses are normalized using the maximum streamwise velocity recorded by the 2DBE model. A. Streamwise turbulence intensity. B. Vertical turbulence intensity. C. Reynolds stress	36
4-1	Riverbed in Guali River - Colombia (a), schematics (b) and velocity profile (c) for a free surface flow over a permeable bed. The velocity at the interface is not zero but it is damped proportionally to depth.	39
4-2	Velocity vector map of the results obtained when implementing the Drag-NS model (a) to a cavity type experiment and its equivalent proposed model (b)	42
4-3	Angle deviation and magnitude discordance (a) and pressure field difference (b) of the velocity vectors calculated from the proposed model and the equivalent Drag-NS model	43
4-4	Computational domain for simulating flow over dune-shaped bed forms from the laboratory setup	44
4-5	Velocity profiles for different values of apparent viscosity and drag coefficients	45
4-6	Velocity field calculated for a porous region represented by (a) $\nu_{ap} = 1$ and (c) $A_d = 10^5$, $B_d = 10^5$. Detailed windows for each case are shown in (b) and (d) respectively	46
4-7	Scalar transport simulation results for dye penetration into porous dunes represented by (a) $\nu_{ap} = 1$ and (b) $A_d = 10^2$, $B_d = 10^2$	47
4-8	Dye injections performed by Fox et al. (2014). Patterns from neutral case are compared with numerical experiment from figure 4-7	48
5-1	Conceptual model. Left: Sand bed with dune-shaped bedforms. The blue box outlines the model domain (λ is the characteristic dune's wavelength). The cyan dashed line demarcates the mean height of the bed. Right: Zoom of the model domain. Idealized streamlines from velocity profiles. Note that the lateral boundary conditions of the model are periodic. Particles (pink rectangles), are seeded at the top of the domain in the left half of the dune, propagate through the bed, and are filtered within bed sediments. The domain is divided into four locations (L1 to L4) to compare the deposition patterns with the experiments from Fox et al. (2018).	55

5-2	Streamlines for Losing (A), Neutral (B) and Gaining (C) flow conditions. Domains are plotted in the interval $[-\pi/2, \pi/2]$ as each domain is periodic. The color bar represents the magnitude of the velocity vector. Vertical and horizontal axis not to scale.	58
5-3	Logarithm of the total number of particles deposited for different times (rows), and under different inflow/outflow conditions (columns). (A) Losing condition, (B) Neutral condition and (C) Gaining condition (Note that axis are not to scale).	62
5-4	Behavior of escaped (dashed Red line), moving (solid blue line), and filtered (dotted green line) particles over time. (A) Losing condition. (B) Neutral condition and (C) Gaining condition.	64
5-5	Residence time function for the different imposed flow conditions. The lines represent the complement of the Cumulative Distribution Function ($1 - CDF$) of particles inside the domain at a time t^*/θ after the injection.	65
5-6	Derivative of RTF for the three vertical groundwater flow conditions modeled. These lines represent the Probability Density Function (PDF) of particles inside the domain at a given time t^*/θ after injection	66
5-7	Comparison with experimental results from (Fox et al., 2018). The top horizontal axis represents the fraction of clay mass found in the experiments expressed in %. The bottom horizontal axis represents the fraction of particles within the numerical domain. Solid colored lines and their corresponding shaded areas represent the average fraction and standard deviation of particles at each depth for the different locations. Crosses are the mean mass fraction sampled in the experiments, and black lines represent the standard deviation of the measurements.	68

1 Introduction

Groundwater - Surface Water (GW-SW) interaction is a research topic that has grown substantially in the latter years. Indeed, the overall quality of river systems is related with the interaction between streams and their underlying aquifers (Cardenas, 2015). Moreover, the place where the interaction occurs, the Hyporheic Zone (HZ) is an extensive research topic by itself (Boano et al., 2014). This topic is not new for science, but it has only been in the last two decades that different advances in the understanding of this zone has been made from the scientific community. The mentioned advances in knowledge about Hyporheic Zone (HZ) and Hyporheic Flow (HF) cover topics that encompass river corridor's ecological state such as water quality, pollutants attenuation, biogeochemistry and river restoration, among others. For instance, HZ and river beds are places where around 80 % of the river biota exists because of its high contents of dissolved oxygen and nutrients contributed by the stream water and the groundwater respectively (Winter et al., 1998). Furthermore, when talking about water supply, GW-SW interactions are a key aspect to manage efficiently water resources and to minimize the impact of extracting water from ecosystems to supply different activities. These interactions are triggered by the river morphodynamics, geology and topographical aspects, showing that a river is not a pipeline and that the water that flows through the stream can leave the main channel and flow through porous media (Vogt et al., 2010). Thus, water from streams can recharge an aquifer or return to the stream later. However, this process influences water quality and acts as a filter where suspended and dissolved pollutants are trapped, adds or removes different nutrients and ions according to the geology of the zone, and finally promotes the existence of ecotones in the river ecosystem.

HF and HE occur from the pore size scale to the whole river corridor, i.e. length, time and velocity scales span within several orders of magnitude and specific physical processes determine the outcome of the exchange. Thus, understanding these complex interaction lead to controversial results that are closely related to the scale in which experiments are made (Boano et al., 2014; Ward and Packman, 2019). Recent hydrodynamics advances focus on small scales (pore size scale and flume experiments), and aim to understand the effect of turbulent mixing in the Sediment- Water Interface (SWI), as well as determine stresses flow features (Roche et al., 2018; Lian et al., 2019). Nevertheless, these experiments and models are made under specific circumstances and cannot be generalized (Ward and Packman, 2019).

For the case of high mountain rivers, HF estimation and hydrodynamics of the SWI are key aspects to understand pollution, nutrient cycles water supply and even risk management (Bencala, 2000; Cardenas, 2015). While water flows through porous media, several biogeochemical processes take part and the ecosystem state influences water quality (Winter et al., 1998). For instance, degradation of heavy metals and organic matter happen within the HZ.

Nonetheless, our ability to determine HF has been a problem and there are no specific expressions to characterize mean flow, or even extreme flow conditions like the ones present in high mountain streams. Only physical experiments made under controlled conditions and with limited geometries have been performed and their results, to the best of the author's knowledge are not conclusive yet (i.e. Pokrajac and Manes (2009); White and Nepf (2007); Pokrajac et al. (2007); Voermans et al. (2017)). In addition, numerical models with high computational demand have been performed (Lian et al., 2019), but their use in everyday situations remains a challenge due to intensive computational resources usage.

Traditional approaches to study HF take into account two different flows, i.e. a free surface flow and flow in porous media. This allows scientists to estimate the exchange between systems using two well-known governing expressions that are widely used in hydrodynamics problems: Navier-Stokes Equations for free surface flow and Darcy's Law for flow in porous media (Cardenas and Wilson, 2007a). These two equations are connected by different means using different boundary conditions and the flow is solved first for the free surface flow and later for the porous media. However, this representation of the phenomena does not take into account that sudden changes in one of the media studies can affect the other one immediately. Also, it does not take into account that the expressions used for describing the water flow have limitations and that HF, specially in highly porous media, goes out of these limitations. For instance, the turbulence effects in the free stream are not transferred to the porous media. Thus, mixing processes within the HZ are not modeled accurately due to the lack of turbulent mixing, observed in different experiments (Fox et al., 2018; Roche et al., 2018). Moreover, limitations regarding the size of the computational domain that can be used for the simulations arise, since only laboratory scales can be handled in this way. Consequently, different model has to be used when dealing with real scale environmental cases.

Therefore, HF lacks of a general governing law, instead a set of different physically based equations are coupled to understand its dynamics. In particular, the superposition of expressions can lead to inconsistencies when talking about conservation of physical quantities like mass or momentum (Cardenas and Wilson, 2007c). Moreover, the transition between a fully turbulent flow in a stream and a complete laminar flow in porous media is not physically possible unless there is a transition zone, suggesting the existence of a porous region with turbulent flow ($Re > O(10^1)$), which cannot be modeled using Darcy's Law (Bear, 1975). In other words, the lack of a governing expression for HF presents a problem to quantify it and consequently to understand the transport, pollution and nutrient cycle phenomena present in this zone. The main soft spot is that there is not a truly physically based governing equation to represent these flows; most of the approaches are *models* to represent those HF processes, which make use of physics based expressions.

Despite the lack of hydrodynamics understanding, the growth of scientific knowledge of the HZ has gathered different areas of knowledge and shifted the traditional physical view to process based domains where different physical features impact the exchange of matter, momentum and energy between free surface and porous media flows, i.e. Hyporheic Exchange (Montgomery, 1999; Ward and Packman, 2019). Such process based domains are defined by

geological, topographic, biological and chemical features, each one of them having different effects on different scales. This approach fosters understanding of HZ and HE; nevertheless, the lack of physical understanding of flow and transport remains a challenge for researchers nowadays. Moreover, connection between different process domains is also not well understood, since single point measurements are not clearly related to higher scales as one currently would expect, e.g. González-Pinzón et al. (2015).

This research aims to explore in detail hydrodynamics of GW-SW undamental processes that can be applied to high mountain rivers, like the ones found in the Colombian Andean region. The research question that is appointed in this document can be synthesized as: *is there a governing law to represent Hyporheic Flow from the physical perspective to characterize and quantify it in a determined portion of a stream in a simplified way?* To address this question, this research proposes as its main goal to test different mathematical models and assess their suitability to represent Hyporheic Flow via numerical models with different advanced techniques.

The motivation for this research topic is to improve scientific knowledge in the field of Hyporheic Flow to address different problems of river ecosystems. To be more precise, our results can be integrated in different strategies of contaminant and nutrient transport or sediment deposition. Moreover, the applications of these results can aid the construction of parsimonious mechanistic models to enhance our ability to understand and manage water resources. To answer the research question, three specific objectives are proposed: *i)* develop different conceptual models to represent in a simplified way the Hyporheic Flow process, *ii)* implement the aforementioned conceptual models into numerical schemes, and *iii)* compare the numerical model with experimental results to evaluate their performance as a hydrodynamics process portray.

To tackle the first specific objective, **Chapter 2** presents the theoretical framework and state of the art in HF and a collection of numerical schemes used for this project. This brief literature review covers the different approaches to the hydrodynamics of HF, the scale that this research aims to solve, a conceptual model for HF and the basic physical processes taken into account. Also, **Chapter 2** presents the main features of the numerical tools used during the current research. This section serves as the main foundation for the discussions of the following chapters. The following chapters are presented as stand alone documents, each one with its own introduction, methods results and discussion following a typical academic paper structure.

Chapter 3 presents our first approach to HF by using the Burgers' Equation to model velocity attenuation in a homogeneous bed composed by spheres packed in a repetition of a cubical array. Here, a Spectral Multidomain Penalty Method (SMPM) is used as the numerical scheme to model a flume bed as a continuum to replace the discrete geometry of pores (second specific objective). Two approaches are used in this experiment, *i)* an apparent viscosity that hinders flow and *ii)* flow modeling through the imposition of Boundary Conditions (BC) from a tested LES model (Lian et al., 2019). The main goal of the chapter is to propose a simplified model to explore and describe flow through the SWI and turbulence dissipation in porous media. Our results are later compared with experimental setups recognized in HF

literature (third specific objective).

Chapter 3 results show that non-linear terms and apparent viscosity play an important role but are not the main flow driver when compared with flume experiments. Therefore, **Chapter 4** explores the use of the full Navier-Stokes Equations to take into account pressure effects in the domain. For this experiment flow equations are modified to take into account the effects of porous media by the use of different viscosity values and drag coefficients (Valdés-Parada et al., 2013). The aim of this chapter is to propose the use of commercial open-source software to represent hyporheic flow. Once again, the numerical models proposed were compared with real case scenarios accomplishing specific objectives *ii*) and *iii*).

To expand our knowledge on HF/HE and to contribute with novel knowledge in GW-SW interactions, **Chapter 5** explores the effects of deposition and filtration of colloids in sand beds under losing and gaining flow conditions. For this purpose, a numerical Particle-Tracking model is implemented using the Advective Pumping Model and a first order filtration, to describe fine particle deposition in rivers with fine grain beds. In a nutshell, this experiment shows that clay deposition in sand beds is controlled mainly by the flow conditions and filtration.

To wrap up, **Chapter 6** presents this research main takeaways, its outcome and a brief discussion of topics for future research. This chapter aims to link the findings of all of the previous sections, discuss them, point their strong and weak points, and discuss future steps in the groundwater surface-water interaction field.

2 General Outline

This chapter presents a the state of the art of HF. Firstly, the physical features and classifications of groundwater - surface water interactions are presented to state this research's domain of interest. Following the scale discussion, fluid mechanics expressions are presented and linked to HF. After presenting the main governing expressions, this chapter discusses the different HF modeling techniques and their up and downsides. Finally, this sections presents a brief discussion about the numerical techniques used to model HF and their utility within the scope of this research project.

Hyporheic Zone was first defined in 1959 by Orghidan. The term “Hyporheic” comes from the antique greek, and combines the prefix “*hypos*”, which means “under”, and the root “*rheos*” that means “flow”. This term highlighted the presence of an important and rich ecosystem under the bed of rivers due to the mixing of surface and groundwater. Nowadays, “Biologists define this zone as the subsurface inhabited by stream macro-invertebrates, hydrologists define the zone as a flow-through subsurface region containing flowpaths that originate and terminate at the stream, and geochemists define it as a mixing zone between surface water and deep-sourced groundwater” (Gooseff, 2010). Bencala defines Hyporheic Zone as “part of a continuum of stream - catchment connections between stream water and soil water, root-zone water, riparian water, quick-flow, delayed flow, macropore flow, and so on to including base flow”. Another useful definition of the HZ is the water that is exchanged back and forth from a surface-water body and the streambed. However, the definition of HF is strongly scale dependent.

Flow along the Hyporheic Zone is the result of different factors that change within a stream, it defines the whole River-Corridor Exchange of matter, momentum and energy between surface water and groundwater (Ward and Packman, 2019). As a consequence, prediction and management within the river corridor is extremely hard to quantify for hydrologic science. This complication arises from identifying that factors such as geomorphology, topography

and climate are the main drivers of the GW-SW interactions (Gooseff et al., 2006). However, human activities, presence of biological communities, and seasonal weather variations can also modify this flows. As a result, scientific community has not found common ground in key topics regarding river corridor exchange at different scales.

For example, water that leaves a stream through its bed travels either short paths in short times and length scales corresponding to the pore scale; or it travels long paths in long time scales. Therefore, different physical phenomena are present and drive different processes along the river corridor, such as biofilm growth, sediment deposition, river bank filtration and nutrient cycling, among many others (Boano et al., 2014; Barthel and Banzhaf, 2015; Roche et al., 2016; Drummond et al., 2017). Several studies have tackled these different processes in the last 30 years, but hydrologic science still lacks understanding of general theories and it is taken merely as a collection of specific case studies (Boano et al., 2014; Cardenas, 2015; Ward and Packman, 2019). Therefore, it is important to acknowledge the different scales or domains that are used in the River Corridor Exchange processes and what are the main drivers within each one of them.

2.1. Domains/Scales within River Corridor

The Process Domain Concept hypothesis is based on the assumption that geomorphic variability dictates the disturbances and processes in different temporal patterns within the riverine ecosystems (Montgomery, 1999). The main idea of the Process Domains is to provide a representation of spatial differences for the disturbance regimes that constitute the river ecosystem. Therefore, within different domains, different processes are relevant and others are considered constant or not driving any biogeochemical disturbance. For the case of GW-SW interactions, several studies have considered different drivers and processes present among different scales (Boano et al., 2014; Barthel and Banzhaf, 2015), in which the HF is studied and to the aim of diverse research fields the HZ can be defined from some centimeters to hundreds of meters, kilometers or even hundreds of kilometers (Buss et al., 2009). For instance, when talking about Ecology and riparian organisms, a point-scale is used, when talking of the scale used to study hydrological features, it may be local, and the scale used to capture hydrogeological phenomena like interactions between regional groundwater flows and surface water bodies is generally regional (Barthel and Banzhaf, 2015). Figure 2-1 shows a schematic view of the three scales that can be used to study the GW-SW interactions that can be associated with domains where processes are driven by different geomorphic features.

The Process Domain that is studied in this research project corresponds to the scale between the grain domain and the channel feature domain. Here, the drivers of the processes are the exchange of mass and momentum through heterogeneous media. This scale is comprised between the Biogeochemical scale and the Hydrologic scale and in this work will be called “hydrodynamical” scale. Our main assumption for working within this scale and processes is that the phenomena studied can be represented using the classical fluid mechanics expressions that govern water flow and transport. Some modifications to the classical expressions can be found in this scale to represent processes that behave far from ideal physics, but the

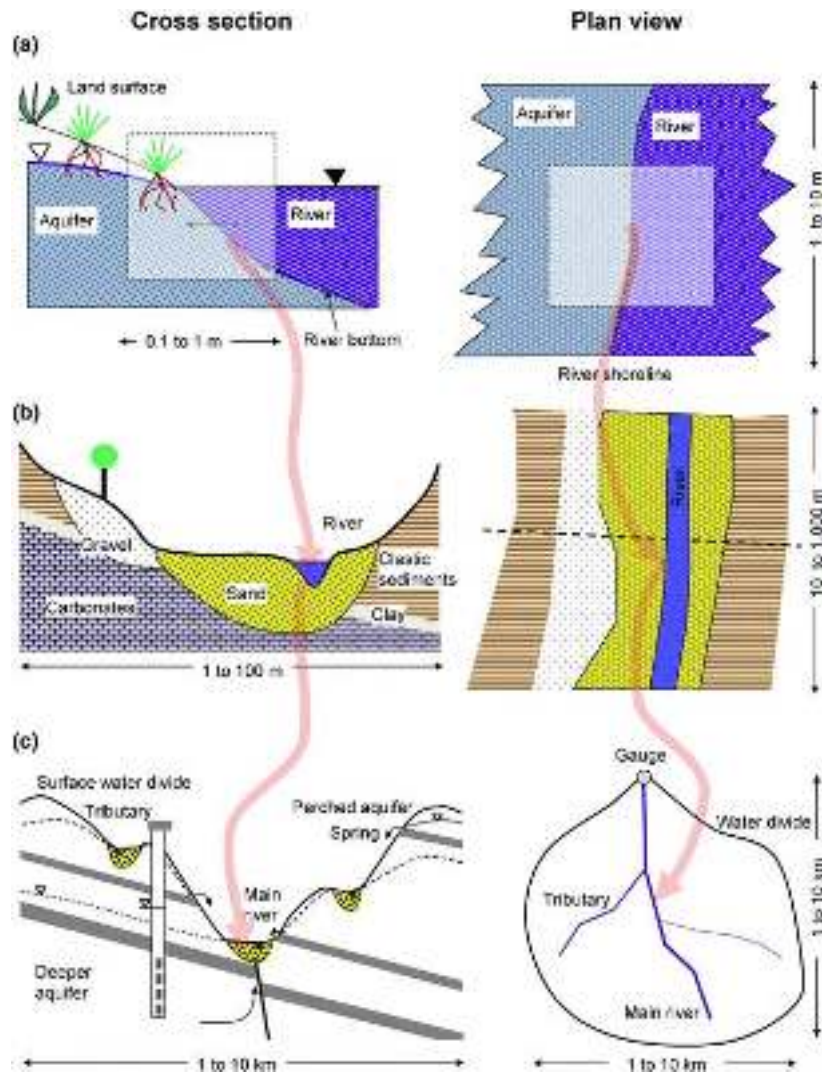


Figure 2-1: Cross section and Plan view of different scales of GW-SW interactions. From: Barthel and Banzhaf (2015).

continuum approach is always applicable. Thus, the equations that govern these phenomena are the expressions derived from mass and momentum conservation laws, i.e., Darcy's Law and Navier-Stokes Equations (NSE).

When studying HF in bigger scales ($O(10^3 \text{ m})$ and higher), the hydrodynamics expressions become unmanageable and the problem has to be tackled from a different point of view. Consequently, hydrological expressions and tools are used to account for a mean change in the whole area studied. However, some changes as depositional patterns of fine sediments, produced by HF in different zones become negligible as the time scale grows. This effect is presented in the work of Bernal (2014) when studying the residence time of water between a lentic surface water body and the aquifer underlying it. The different scales managed and, their approaches and their association with geomorphic processes are discussed in the three following section.

2.1.1. Hydrogeological Scale - Geological and Lithotopo Processes Domain

The Hydrogeological scale studies the GW-SW interactions in a broad scale and its Processes Domain Controls are those associated with the geology and geomorphics of the river corridor that is being studied. In fact, its object of study focuses in regional flows and the possible links between basins due to their connection with common aquifers. Moreover, this scale takes into account complex geology due to the scales used in space (i.e. broader than $O(10^3 m)$), and its study is subject to different techniques like geochemistry and isotope hydrogeology (Buss et al., 2009). In this scale, the aforementioned processes dictate the shape of the basins, landscape evolution and presence of different ecosystems (Ward and Packman, 2019). In terms of physical quantities, this scale takes into account mass conservation, neglecting momentum and energy conservation.

Figure 2-2 shows a conceptual example of the areas studied by the Hydrogeological Scale of HF. However, this scale is not inside the aims of this research because the it is not possible to cover it with hydrodynamics models like the ones proposed for this research.

2.1.2. Hydrological Scale - Reach Domain

This scale covers River Corridor Exchange from tens of meters to values close to the thousands of meters (i.e. from $O(10^1 m)$ to $O(10^3 m)$) and it can be used either to study typically water balances using mass conservation, or momentum conservation in environmental flows. However, the length scale covered in the hydrological scale can have two different approaches. The processes associated with this scale are dominated by the lithotopographical units that constitute a hydrological basin. More specifically, the HF quantification and characterization can be done with an approach based on hydrodynamics and physically based processes, or with an hydrological approach that takes into account the storage in different zones of the area studied in order to build a “Water Budgets” based on mass conservation exclusively. Figure 2-3 shows the phenomena that the Hydrological scale is able to capture.

Nevertheless, the hydrological scale lacks the ability of capturing phenomena driven by hydrodynamics, form features and complex media. This scale does not capture phenomena under the $O(1day)$ scale and under $O(10m)$ length scale. Therefore, the current research does not use this scale. Indeed, the scale that is going to be used is called hydrodynamics scale and it is explained below.

2.1.3. Hydrodynamics or Ecological Scale - Feature and Grain Processes Domains

This scale is characterized by a small size. Indeed, its order of magnitude goes from $O(10^{-3} m)$ or less to units of meters ($O(10^0 m)$), and its time dependency can go from a fraction of a second to days (i.e. between $O(1 s)$ and $O(1 day)$). The HF Biogeochemical scale is used mainly to study changes in water quality due to the presence and transport of nutrients

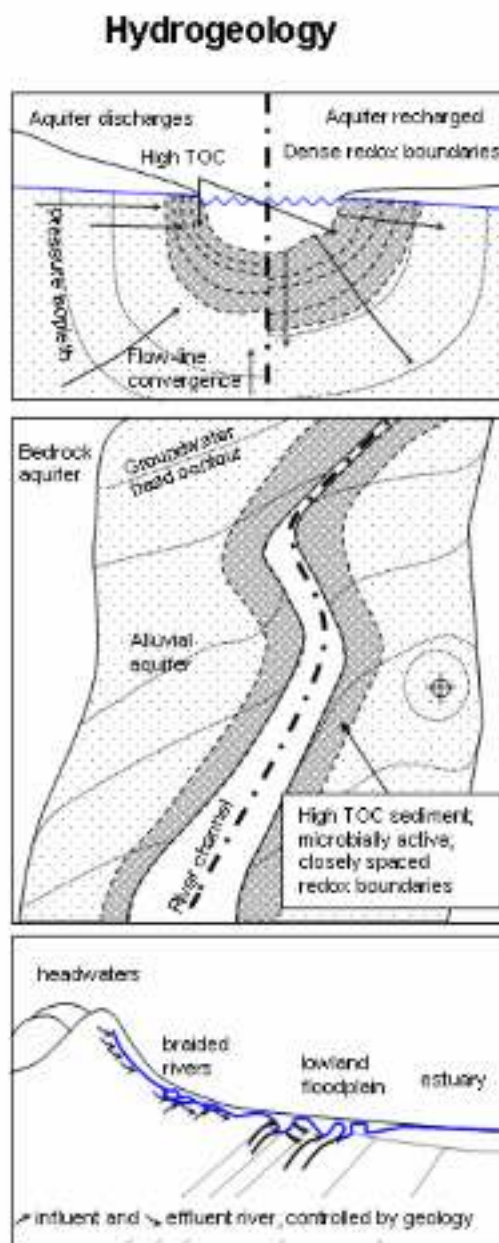


Figure 2-2: Conceptual model of Hydrogeological scale. From: Buss et al. (2009)

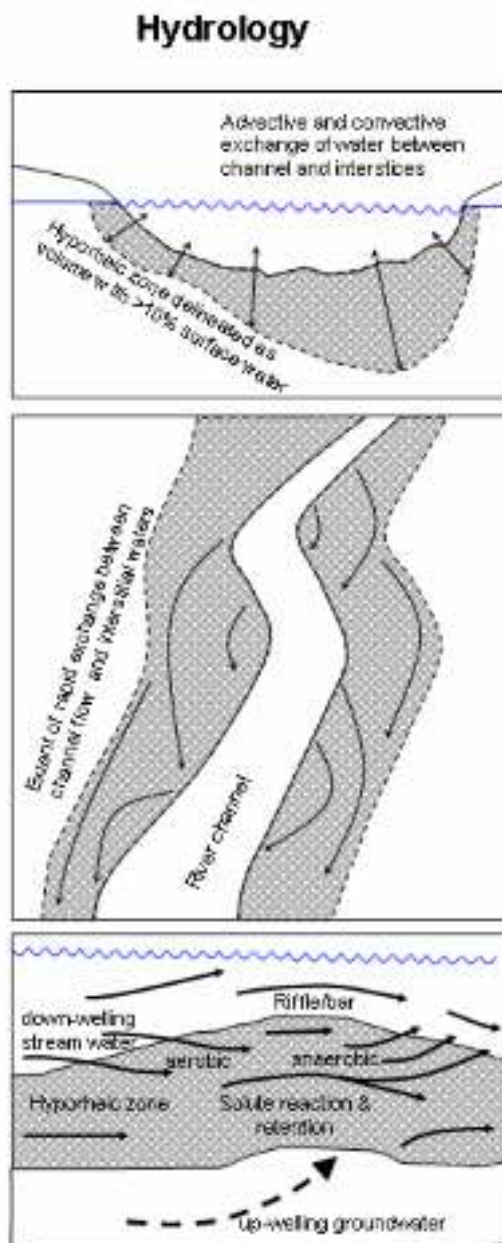


Figure 2-3: Conceptual model of Hydrological scale. From: Buss et al. (2009)

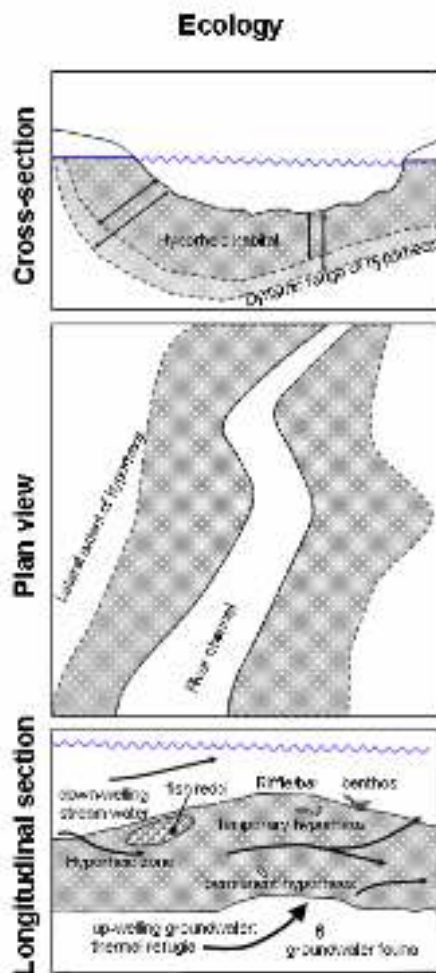


Figure 2-4: Conceptual model of biogeochemical scale. From: Buss et al. (2009)

and either conservative or reactive components. Figure 2-4 shows a graphic example of the processes studied in this scale (Buss et al., 2009). Here, the governing equations from hydrodynamics and transport can be used to explain different phenomena driven by mass, momentum and energy exchange between the river and the surrounding porous media.

The topics studied using this approach or scale comprise benthic fauna, fish population and spawning, contaminant transport and nutrient cycles inside the HZ. Although in some cases these topics include flow study, the biological and chemical reactions are more important for this scale of study. However, the approach from the hydrodynamic point of view is necessary to fully understand the transport processes in scales between centimeters and a few meters (i.e. from $O(10^{-2} \text{ m})$ to $O(10^1 \text{ m})$).

This scale relies in the explanation of water movement in order to characterize and describe flows. Unlike the hydrological scale, which only accounts for water mass balances, this scale takes into account water velocity and momentum to understand how the phenomena occurs (Paiva et al., 2011). In addition, the hydrodynamics scale can be used also to observe changes

in water quality, which are hard to capture in an hydrological scale, but can be detailed better if the biogeochemical scale is used.

This scale order of magnitude in space goes from $O(10^{-3} \text{ m})$ to $O(10^2 \text{ m})$. Besides, it takes into account the dynamics of the rivers (research's object of study), which is not taken into account by the hydrological scale approach. Also, the hydrodynamics scale can represent phenomena with small temporal variation (i.e. $O(1 \text{ s})$ to $O(1 \text{ day})$), that is hardly reproducible with hydrological models, as shown by Bernal (2014).

In brief, the hydrodynamics scale is based in the physical phenomena and the processes within it are governed by topography, slope and grain size of the river that is being studied. Here, the lithological composition is important but can be taken as constant along the study domain. Therefore, this scale uses water mass balances, like the hydrological one, and it also uses momentum conservation law and flow equations derived from the conservation laws discussed in section 2.2. Because of the reasons mentioned above, this scale is the one selected for the development of this research project.

2.2. Fluid Dynamics and Hyporheic Flow

The understanding of HF from the physical point of view requires as a first input the basic expressions that rule the flow of water in two different media, i.e. free surface flow and flow in porous media. These governing laws were proposed during the eighteenth and nineteenth centuries in Europe by scientists and engineers like Euler, Navier, Stokes and Darcy among others and aimed to explain the conservation of three main physical quantities: mass, momentum and energy. Since this research looks for a governing expression that characterize and quantify HF, these expressions are going to be used as inputs for the research development. In 1755 Euler derived the equations that described the “frictionless” motion of incompressible fluids. Later Navier (1827), Poisson (1831), Saint-Venant (1843) and Stokes (1845) deduced the fluid dynamics equations that are widely used today in the study of fluids (Ruban and Gajjar, 2014). These expressions have been used for over two centuries for explaining the phenomena studied by Environmental Fluid Mechanics (EFM). In the beginning, there was a close bond between experimentation and theoretical reasoning. However, the current use of computers and complex algorithms have included Computational Fluid Dynamics (CFD) to the study of water flow.

The expressions that rule fluid motion are derived from “*conservation laws*” and provide a description of the fluid's behavior under certain circumstances (Kuzmin and Hamalainen, 2015). Indeed, the general form of the conservation laws state that the rate of change of a fluid property can be expressed as the sum of the inflow, outflow, sources and sinks inside the control volume selected to do the analysis. This research aims to use the existent fluid mechanics theory to find an expression that can describe HF in high mountain rivers. In order to accomplish this objective, the mass and momentum conservation are going to be used. Table 2-1 shows the main equations in their generalized form.

Fluid Property	Equation
Mass	$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$
Momentum	$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \rho \mathbf{g} - \nabla \cdot \bar{\bar{\sigma}} = 0$

Table 2-1: Mass and Momentum Conservation Laws in Fluid Dynamics

In Table **2-1**, ρ symbolizes the fluid density, $\mathbf{u}$ the fluid velocity field, t the time, $\mathbf{g}$ the body forces of the fluid, and $\bar{\bar{\sigma}}$ the stress tensor representing the surface forces. Although the energy conservation law exists, phenomena like heat exchange is not taken into account in the aims of the research. Based in the expression shown in Table **2-1**, the Navier-Stokes equations and the Darcy's Law for flow in porous media were developed. Table **2-2** shows the expressions of flow under laminar conditions and not taking into account the effects of turbulence. Both expressions shown in Table **2-2** govern incompressible flow, Navier-Stokes for free surface flow, and Darcy law for flow in porous media.

Flow Equation	Equation
Navier-Stokes	$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \mu \Delta \mathbf{u} + \nabla p = \rho \mathbf{g}$
Mass conservation	$\nabla \cdot \mathbf{u} = 0$
Darcy Law	$-\bar{\bar{K}} \frac{\partial h}{\partial x} = \mathbf{q}$

Table 2-2: Basic Flow Equations for the research project

In Table **2-2**, h represents the hydraulic head of the fluid in the porous media, and K represents the Hydraulic Conductivity of the media where the fluid is moving. The other symbols used in the equations of Table **2-2** are the same used for Table **2-1**.

The expressions for flow in porous media were later used by Vaux in 1968. He developed a one dimensional mechanistic model that combined the inflow and outflow of water inside a control volume of porous media (Vaux, 1968). The model proposed suggests that the HF is driven by spatial changes of energy in the system, shape change of the bedform and changes in the conductivity of the porous media. The schematic of the proposed model is shown in Figure **2-5**, and the mathematical form is shown in Equation 2-1, where "e" stands for the total exchange of water in the control volume.

$$e = -KA \frac{d^2 h}{dl^2} - K \frac{dA}{dl} \frac{dh}{dl} - A \frac{dK}{dl} \frac{dh}{dl} \quad (2-1)$$

Where K stands for the media's Hydraulic Conductivity, h for the total head of the flow, A for the area where the flow is passing and l for the longitudinal direction considered. The

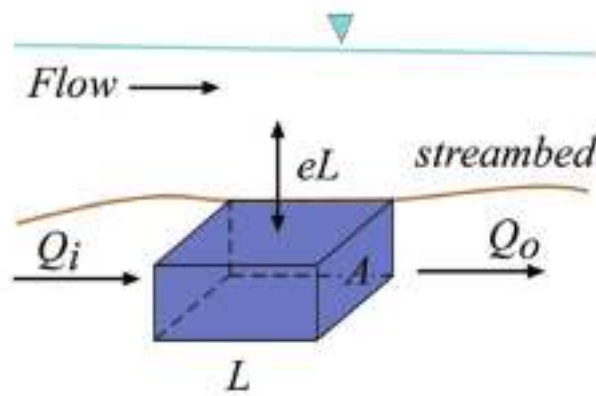


Figure 2-5: Conceptual model of Vaux proposition for HF. From: Tonina and Buffington (2009)

expression shown in Equation 2-1 is quite simple, but it gives a merely physical approach to the HF phenomena in ideal scenarios. Nevertheless, it can be modified in order to account for heterogeneity, temporal variation of properties and different flow regimes. However, Vaux supposed that HF was laminar, since he used the Darcy Law for flow in porous media.

Another approach taken by the current HF researchers is its quantification using the the Advection Diffusion Equation (ADE), presented in equation 2-2. The term "k" in this equation stands for the different approaches and modifications made to the original ADE proposed for transport in media with no temporal storage or dead zones like rivers. This approach is widely used by the scientific community nowadays. However, in theory the velocity distribution used for this equation comes from solving the flow equations. Consequently, it is useful to know first the flow patterns, directions and magnitudes before applying any transport model. The ADE in its generalized form is expressed as follows,

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = D(\Delta C) + k, \quad (2-2)$$

where C stands for the concentration of a conservative tracer, t for time, $\mathbf{u}$ for the velocity field D for the dispersion coefficient. As it was discussed in section 2.1, the main driver for large scales is the hydrostatic pressure, and so it is called "Hydrostatic HF". Meanwhile, at small scales the HF is driven mainly by Hydrodynamic Pressures, and thus it is called "Hydrodynamic HF" (Boano et al., 2014). Moreover, the drivers that trigger HF in large scales are related with climatic and meteorologic influences, i.e. they have to be taken into account with an hydrological approach rather than with a pure physical one.

Our research presents a figure modified from Boano et al. (2014) (figure 2-6), where different factors and scales are presented to understand HF in all its extent (Boano et al., 2014). The left part of the figure contains the hydrodynamic drivers of HF, while the right part shows the hydrostatic drivers. An important part of the graphic is the relationship between the HZ

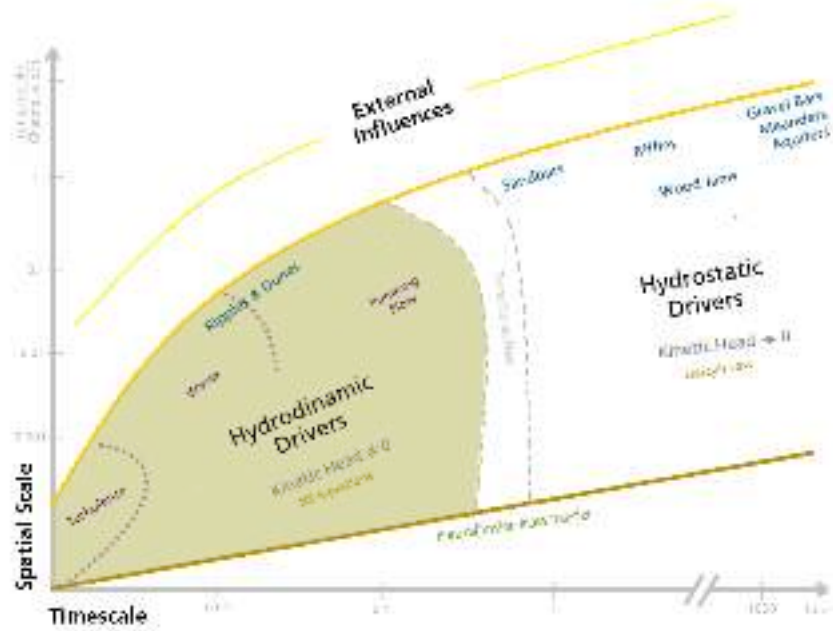


Figure 2-6: Spatial and temporal timescales for SW-GW interaction. Adapted from Boano et al. (2014)

and the channel width, that defines the "y" axis of the graph. As it was mentioned before, as the scale grows up (from $O(10^2 \text{ m})$), the HF drivers tend to be influenced by climate, so the hydrological approach becomes relevant in front of the pure physical approach.

2.3. HF Models: State of the Art

Since the proposed research aims to build a modeling framework of HF in high mountain rivers, it is necessary to review the models used nowadays to explain this phenomena in different stages. Therefore, this section will explain the conceptual models used, the governing expressions used and their strengths and weaknesses. The first model to be discussed is the applied mathematical model proposed by Discacciati et al. (2002), in second place the one proposed by Cardenas and Wilson (2007c), thirdly, the one used by Higashino and Stefan (2008) and modified by Peñaloza-Giraldo et al. (2015); another model is the one proposed by Huang et al. (2008) used mainly for oceanography, but with similar behavior in rivers; and finally the conceptual models for numerical Particle-Tracking are discussed using the one proposed by Li et al., and used in this research project in chapter 5.

2.3.1. Coupling of Navier-Stokes and Darcy Law

The models proposed by Discacciati et al. (2002) and Cardenas and Wilson (2007a) have in common the use of the equations of flow in free surface and porous media in order to quantify the flow in a determined area of interest, i.e. the HZ (table 2-2). This model defines two

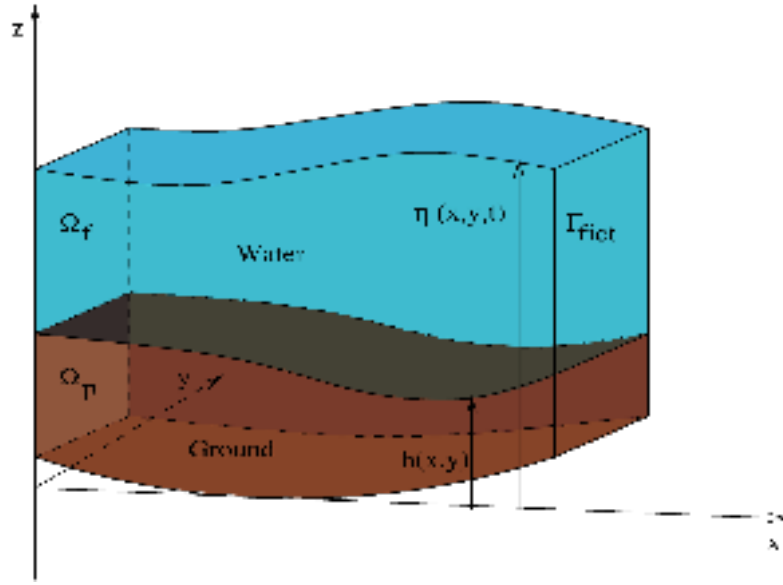


Figure 2-7: Conceptual domain adapted from: Discacciati et al. (2002)

domains, each one of them ruled by a different flow equation. Figure 2-7 shows a schematic of the model used, where Ω_f represents the river, and Ω_p represents the porous media.

The proposed model solves the Three Dimensional Navier-Stokes Equations (equation 2-3, defined in table 2-2) for the domain Ω_f . The boundary conditions applied to this part of the model are flow velocities and pressures are imposed in the faces as shown in Figure 2-8. Velocities are designated with Γ and Pressures with Λ . However, the particular issue of this model is how does it propose the velocity continuity in the boundary between the free flow and the porous media. In this case, the velocity normal to the bed is equal in both domains and the tangential velocity can change. Regarding the pressure, it is continuous in the two domains (Discacciati et al., 2002). Then, Darcy's law (equation 2-4 defined in table 2-2) is solved to obtain the total flow field.

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \mu \Delta \mathbf{u} + \nabla p = \rho \mathbf{g} , \quad (2-3)$$

$$-\overline{K} \frac{\partial h}{\partial x} = \mathbf{q}, \quad (2-4)$$

Discacciati et al. (2002) model is merely theoretical. Its application was proposed for ideal conditions and simple geometries. Its applicability under complex geometries like the one present in mountain rivers is difficult if the meshes used are fine, because of the number of calculations needed. Besides, the continuity conditions of velocity and pressure between the two domains proposed are difficult to be complied in real cases. As a consequence, Cardenas

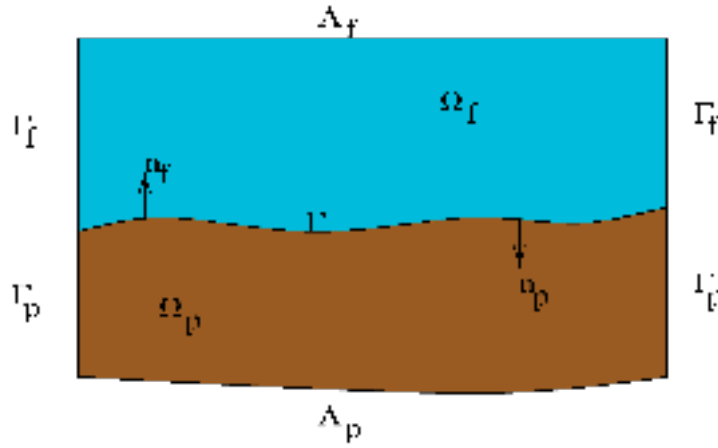


Figure 2-8: Discacciati et al. Coupling model. Adapted from: Discacciati et al. (2002)

and Wilson (2007a) proposed a similar model for calculating HF using the same domains, but different coupling conditions between them.

The first difference between Cardenas and Wilson (2007a) model and the one presented by Discacciati et al. (2002) is the number of dimensions represented. Cardenas and Wilson (2007a) propose two dimensions and the solution showed by Discacciati et al. (2002) is made in three dimensions. The conceptual model used by Cardenas is shown in Figure 2-9.

Both models presented in this section represent the water flow in two different media and take into account the behavior of the free surface flow as an input for the behavior of the flow in porous media. However, they take into account that Darcy Law is applicable all over the porous media, and this assumption has to be revised. As a matter of fact, the use of Darcy Law for turbulent flows in porous media is not recommended and different expressions have to be used in order to estimate water velocity (Bear, 1975).

2.3.2. Velocity Damping Models

The second type of HF models that are going to be discussed rely on the dissipation of velocity in the porous media. Indeed, these models do not use Darcy's Law for describing the flow in the porous media but a modification of the Navier-Stokes equations. This model was used by Higashino and Stefan (2008) and modified by Peñaloza-Giraldo et al. (2015). However, in both cases the water velocity was simulated as a perfect one period wave, rather than a real velocity signal captured in real case scenarios.

Moreover, these models worked in one dimensional cases, thus their extent for quantifying HF is limited and they should be extended to at least two dimensions. The vertical velocity pulse used by both models is presented in Figure 2-10. In the case of Higashino and Stefan the mean velocity had a value of 1 cm/s , while in the case of Peñaloza-Giraldo et al. (2015)

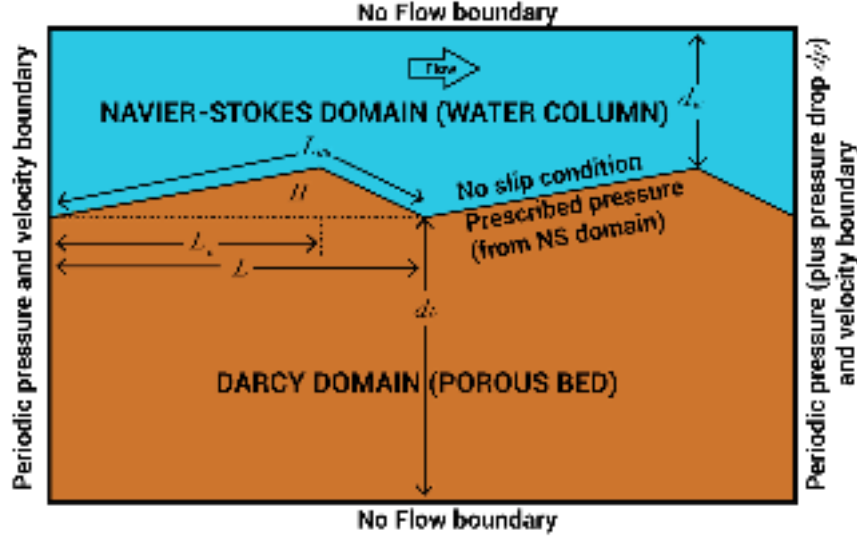


Figure 2-9: Cardenas and Wilson conceptual 2D model. Adapted from: Cardenas and Wilson (2007c)

was 0 m/s.

In addition, both models use spectral methods in order to solve the turbulent velocity damping. The Higashino and Stefan (2008) model uses a Fourier Spectral Method (periodic), while the Peñaloza-Giraldo et al. (2015) uses a Spectral Multi Domain Penalty Method (SMPM). The main difference between these methods is in the boundary conditions. Namely, the Fourier methods rely on periodic boundary conditions, while the Spectral Multi Domain Method does not have that restriction.

The conceptual model from which the discussed models are based is presented in Figure 2-11. The main assumption of the model are that the flow that enters the porous media is turbulent, and that the turbulence is dissipated while water flows down in the domain until it arrives to a mean velocity which is equal to the average flow velocity within the porous media.

The equation solved by the model is a 1D Burgers Equation type, which is a well known simplification of the 1D Navier-Stokes Equations for the vertical coordinate where the Pressure is considered hydrostatic. The Burgers Equation is presented in 2-5. Besides, this equation includes a term called “apparent viscosity” (ν_a), which recreates the velocity drop due to its flow through the porous media.

$$\frac{\partial w}{\partial t} + w \frac{\partial w}{\partial z} = \nu_a \frac{\partial^2 w}{\partial z^2}, \quad (2-5)$$

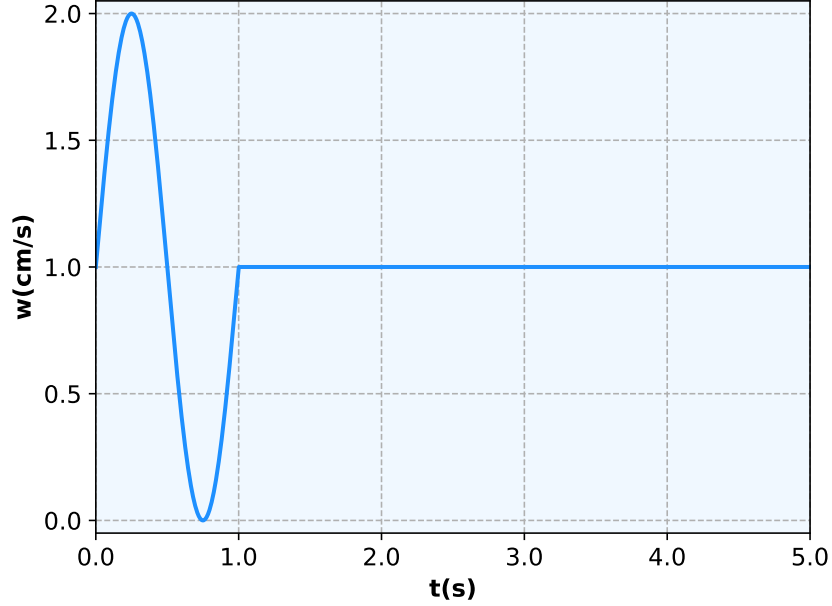


Figure 2-10: Velocity pulse modeled by Higashino and Stefan and Peñaloza-Giraldo et al. Adapted from: Higashino and Stefan (2008)

where w represents water's vertical velocity, z the vertical space and ν_a the apparent viscosity which has to be calculated using the media properties like porosity and grain size of the riverbed. It is important to take into account that this equation does not include the effects of pressure produced by the free surface flow, and that precisely is one of the weaknesses that it shows. However, it is able to recreate the damping of a theoretical function introduced as a top boundary condition. The apparent viscosity (ν_a) mentioned in the Burgers Equation was taken out from the work of Boudreau (1997), and the initial deductions made by Bear (1975). This simplification allows the construction of the coefficient that depends on the grain size of the HZ.

The work done by Peñaloza-Giraldo et al. (2015) was the basis for a real case scenario presented in the EGU 2016 General Assembly by Preziosi-Ribero et al. (2016) in a PICO presentation. In this work, the SMPM was used to recreate the velocity damping in the porous media with real case velocity measurements made in the Gualí River in the Department of Tolima, in Colombia. The main result of the work presented was that the equation used is also able to recreate the velocity damping in porous media, even when using a continuous signal rather than a trigonometrical pulse. However, the only parameter that this equation has is an apparent viscosity that changes due to the media heterogeneity, and has no physical meaning other than the introduction of a term that helps to reduce velocity in the media. Perhaps this equation can be used in rivers with no turbulent flows, but in high mountain rivers the pressure is a driver for HF (Tonina and Buffington, 2009).

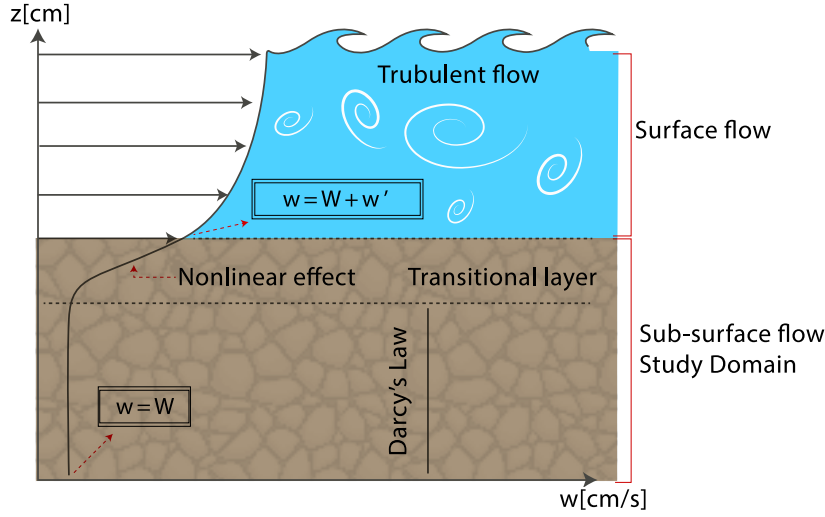


Figure 2-11: Conceptual Model for velocity damping. Adapted from: Peñaloza-Giraldo et al. (2015)

2.3.3. Oceanography Example

The model proposed by Huang et al. (2008) is similar to the one proposed by Discacciati et al. (2002) and Cardenas and Wilson (2007a). Indeed, it differentiates two media and tries to couple them with two different expression. Nonetheless, this model uses two versions of the Navier-Stokes Equations, thus, for the free surface flow it is the one presented in Section 2.2, and for the porous media it uses a modification of the same Navier-Stokes Equations for porous media proposed by Huang et al. (2003), which is presented in Equations 2-6, 2-7 and 2-8.

$$S \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - \frac{\nu n_w}{k_p} u - \frac{C_f n_w^2}{\sqrt{k_p}} u \sqrt{u^2 + v^2}, \quad (2-6)$$

$$S \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \frac{\nu n_w}{k_p} v - \frac{C_f n_w^2}{\sqrt{k_p}} v \sqrt{u^2 + v^2}, \quad (2-7)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (2-8)$$

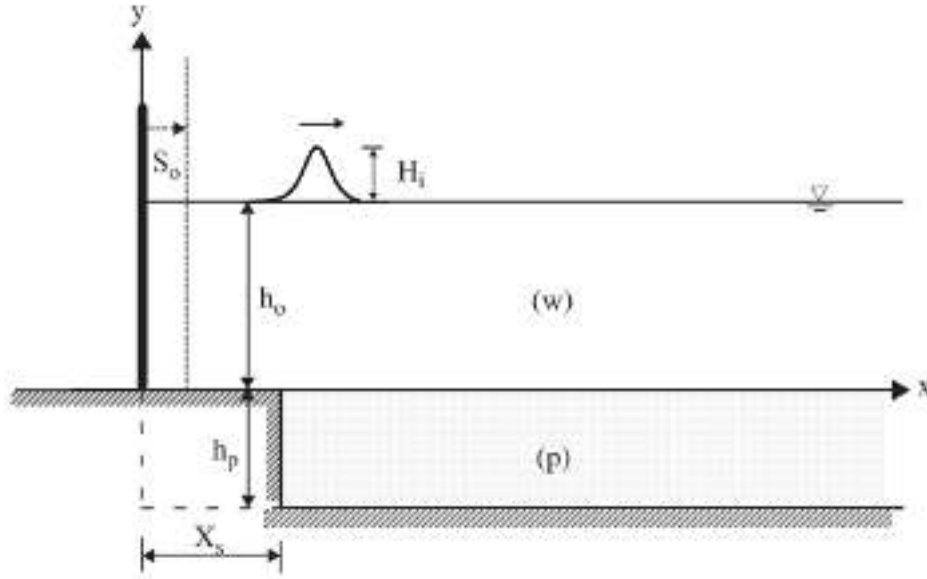


Figure 2-12: Conceptual Model in oceanography. From: Huang et al. (2008)

where k_p is the porous media intrinsic permeability in m^2 , n_w is its porosity (dimensionless), C_f is a dimensionless coefficient that represents the turbulence resistance and S is defined in Equation 2-9, where C_m is a coefficient of added mass.

$$S = 1 + C_m \frac{(1 - n_w)}{n_w}, \quad (2-9)$$

The conceptual model solved by Huang et al. (2008) is the one shown in Figure 2-12. As it can be seen, this model represents a perturbation on the surface of the sea and how the changes in pressure and velocity due to that perturbation affect the flow in the porous media below. Although this approach uses physical equations, the appearance of the dimensionless coefficients C_m and C_f represents a challenge for real measurements, and later on a calibration problem if it is intended to compare its results with a real case scenario.

2.3.4. Numerical Particle-Tracking

The Numerical Particle-Tracking technique is used to study sediment transport and deposition in rivers using the flow fields obtained by some of the methods described above in this section. The numerical Particle-Tracking is based in the Langevin's equation (Eqn. 2-10) as a Lagrangian analogue for the ADE equation, applied to numerical particles that follow flow paths within a prescribed domain and are subject to advection and dispersion processes that are governed by different probability distributions to estimate their total movement. The results are averaged spatially and temporally to obtain continuous fields of deposition (Li

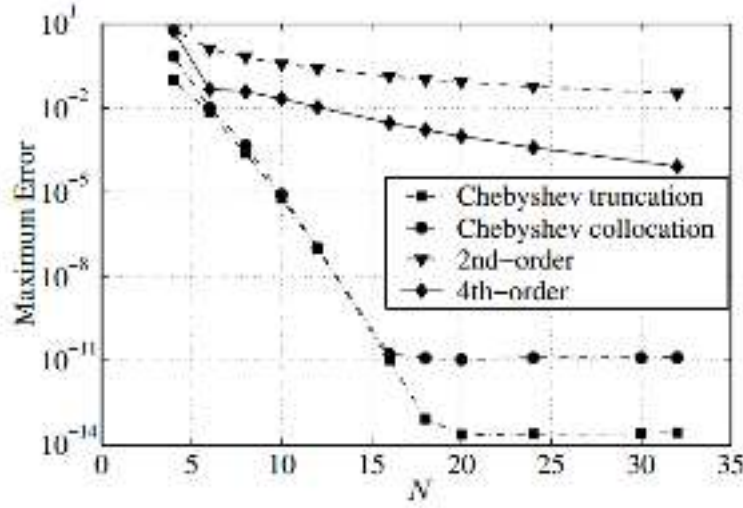


Figure 2-13: Error of collocation method against high order finite difference method. From: Canuto et al. (2009)

et al., 2017; Preziosi-Ribero et al., 2020).

$$x(t + \Delta t) = x(t) + u_x \Delta t + \xi \sqrt{2D_x \Delta t}, \quad (2-10)$$

2.4. Numerical Tools

Regarding the numerical methods, three of them are used for this research. First of all, a method that offers flexible treatment for non linear processes, minimum numerical diffusion and an element based approach is used in chapter 3. Later, in chapter 4 a traditional Finite Volume Method (FVM) is used since its precision is lower than the one offered by spectral methods (figure 2-13) (Canuto et al., 2009). For the final approach, a method based on the numerical particle tracking is implemented in chapter 5.

Nowadays, the most used numerical methods to solve equations in fluid mechanics are the Finite Volumes Method (FVM), Finite Differences Method (FDM) and Finite Elements Method (FEM). Indeed, most of the software packages used to calculate solutions to different equations use one of these methods. However, it is out of the scope of this document to explain the basic functionality of these methods, since the idea of the research is the implementation of a Spectral Method: “Spectral Multi-domain Penalty Method (SMPM)”.

In order to review the capabilities of the methods discussed in this section, Table 2-3 shows each one of them and either if it is possible for the method to recreate complex geometries, if it has a high order accuracy (i.e. error lower than $O(10^{-6})$), if it can portray explicitly the discrete form of fluid dynamics equations, if it can recreate the mass and momentum

conservation laws and if it is able to solve elliptic problems. The reference used for the construction of this table is Hesthaven and Warburton (2008).

Table 2-3: Generic properties of most widely used numerical methods

Method Used	Complex Geometry	High Order Accuracy	Explicit Semi Discrete Form	Conservation Laws	Elliptic Problems
FDM	No	Yes with modifications	Yes	Yes	Yes
FVM	Yes	No	Yes	Yes	Yes with modifications
FEM	Yes	Yes	Yes	Yes	Yes with modifications
DG and Spectral Methods	Yes	Yes	Yes	Yes	Yes with modifications

2.5. Summary

This chapter presented an overview of the state of the art regarding HF, its physical basis, the governing expressions and conceptual models. Furthermore, different modeling approaches were discussed, presenting their strengths and weaknesses. Finally, the different numerical techniques that are going to be used in the following sections are presented. The following chapters present the three different modeling approaches applied during this research project, i.e., Burgers Equation with SMPM, NSE with commercial packages and Particle-Tracking using MATLABTM.

3 A Simple Hydrodynamics Profile for Hyporheic Flow

The first approach to simplify Hyporheic Flow is presented in this Chapter by proposing the Burgers' Equation (BE) as a feasible expression. To accomplish this goal and test the suitability of the expression, results from a detailed Large Eddy Simulation (LES) model are plugged into a two dimensional numerical model and the results are compared with experimental data retrieved from flume experiments. BE is proposed because of previous uses in modeling complex phenomena, its ability to represent shock-wave flows and its simplicity for having only one parameter to govern it (Reynolds number in its non dimensional form).

3.1. Introduction

Hyporheic Zone and Hyporheic Flow are becoming hot topics for science nowadays (Cardenas, 2015). The study of this zone and the exchange that happens here is vital to understand the fate of nutrients and contaminants in the river corridors (Boano et al., 2014). Besides, rivers are suppliers of freshwater and discharges' receivers of cities all around the world, and understanding the dynamics between streams and their surroundings is important for governments, academia and general public. However, rivers and their surroundings are complex natural systems with heterogeneous scale-dependent and non linear properties, hence modeling them becomes a great effort that has to be tackled from different sciences and scales as discussed in section 2.1.

Hydrodynamical models developed for HF can be coarsely divided in two groups: (i) Direct simulation models that detail the porous media and free flow to solve Navier-Stokes Equations (NSE) within all of the spaces where water can flow inside the domain; and (ii) simulations that take into account continuous domains and use either physically based governing expressions or simplifications to model Hyporheic Flow. In general, both of this

types of models seek to portray flow and/or transport by solving two different types of flows and coupling them via boundary conditions, that transfer information from one domain to another. Examples of this solutions are found in Hyporheic Flow/Exchange literature using different models, as mentioned in section 2.3.

This section aims to present a simplified expression to model HF using the Burgers' Equation to avoid the problem of solving the full NSE and open the door for solving less complex expressions for HF while retaining to some extent, useful information about the phenomenon studied. To accomplish this objective, a Spectral Method (SMPM) is going to be used in order to have a stable, element based numerical scheme with small numerical diffusion and high order accuracy as shown in section 2.3. Results obtained in this section are going to be compared with physical experiments carried out in flumes with homogeneous and heterogeneous media.

Results from this section suggest that the use of simplified expressions to model HF requires extreme care, since the basics of the processes analyzed can be neglected because of the simplifications used. In addition, the development of models such as the one described in this section requires the developing of a more complex model or intensive data collection from flumes or natural streams.

3.2. Conceptual and Mathematical Model

The proposed model aims to simulate turbulent velocity attenuation within a granular bed comprised by regular spherical beads in cubic packing. This is a common physical model used in experiments that use Particle Image Velocimetry (PIV) in 2D and 3D (Pokrajac and Manes, 2009; Voermans et al., 2017; Roche et al., 2018). However, our model's domain comprises the granular bed and does not take into account the free flow above it. As a consequence, the processes associated with the free surface flow are imposed as boundary conditions at the top of the computational domain. Specifically, it takes as an input the horizontal and vertical velocities at the top of the SWI of a LES model (Lian et al., 2019), a no slip condition at the bottom and periodic conditions on the sides (figure **3-1**). Hence, the hydrodynamic conditions of the flow are fed to the model as velocity signals in different spots. Therefore, this model's output is the instantaneous velocity in different parts within the sub surfacial domain using a non linear transport equation assuming hydrostatic pressure within the whole domain.

3.2.1. Conceptual Model

The primary assumptions within the model are: (i) the hydrodynamic processes can be represented with the expressions of the continuum mechanics; (ii) the velocity at the top of the domain is enough to represent the interaction between the flow and the spherical packed bed; (iii) the geometry of the bed does not change with time, hence the conditions that represent the media properties are constant in time; (iv) the 3D physical process can

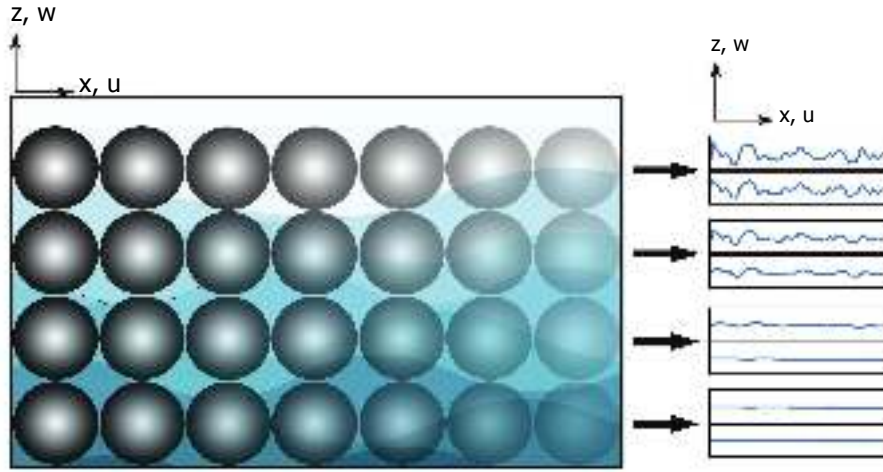


Figure 3-1: Conceptual model of velocity attenuation within an idealized porous media. The velocity over a vertical profile is expected to decay in magnitude and to have a decay in RMS. In this figure x and u stand for streamwise coordinate and velocity and z and w stand for vertical coordinate and velocity, respectively. The conceptual model is an adaptation from Lian et al. (2019).

be averaged in space and a two dimensional model can represent the average behavior of the complex phenomenon; (v) a hydrostatic pressure gradient within the whole domain; and (vi) steady state was considered in the model when the difference between time averaged velocity signals was less than 5 %. In other words, a three dimensional complex process is going to be simplified into a two dimensional domain and the velocities within that domain can be modeled using the BE and the proper boundary conditions. Continuum mechanics are used constantly to reproduce mean flow behavior in porous media (Freeze and Cherry, 1979; Domenico and Schwartz, 1998). This approach is common in physics and aims to simplify heterogeneity and anisotropy of natural media. Therefore, the full flow profile and description cannot be recovered, but the approximation that these models yield are enough in most of the cases to represent physically the phenomenon under different conditions. Moreover, to ensure that there is no influence from the lateral boundaries, our model is periodic in the x direction (figure 3-1). The model's periodicity in the streamwise axis ensures that the phenomenon of flow over the porous bed is representative at a different range of scales and also eliminates the effects of bounding the flow in that direction.

For the current problem, the 2D Burgers' equation (2DBE) is proposed, starting from the incompressible Navier-Stokes momentum Equations (equation 3-1), where w is the vertical velocity, P is the pressure ν is the kinematic viscosity of water and g is the gravity acceleration. When Hydrostatic flow is assumed the pressure gradient $-\partial P/\partial z$ becomes $-\rho g$ and

the pressure term is canceled with the external forces in the vertical direction g .

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial P}{\partial z} + \nu_a \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial z^2} \right), \quad (3-1)$$

Our assumption contemplates that since the domain is small enough, the variations of pressure are considered linear, and equal to the gravitational forces that the fluid is subject to. The 2DBE has been widely used in computational fluid dynamics to simulate wave propagation, viscous flow and turbulence, gas dynamics and it is also widely used to model other physical phenomena (Bonkile et al., 2018). For the present model, the 2DBE is used as the model that propagates velocity signals taking into account the influence of adjacent signals that feed the top part of the domain (equations 3-2 and 3-3).

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial z} = \nu_a \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial z^2} \right), \quad (3-2)$$

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + w \frac{\partial w}{\partial z} = \nu_a \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2} \right), \quad (3-3)$$

The use of the 2DBE for modeling Hyporheic Flow can be compared with a portion of the methods discussed in section 2.3.1, where a free surface flow is solved using the NSE and then the velocity/pressure results at the bottom of the domain are imposed as a boundary condition to the porous media flow. However, since for this case real velocity signals are gathered at the top of the porous media domain, there is no need for solving free surface flow. The aim here is to obtain velocity signals that are more realistic than the averaged results that are obtained in the use of averaged equations (Discacciati et al., 2002; Cardenas and Wilson, 2007a). However, the author acknowledges that the current approach does not ensure mass conservation, since there is not an equation to ensure it without over constraining the proposed system.

3.2.2. Numerical Model

The numerical scheme selected to solve the 2DBE was a Spectral Multidomain Penalty Method (SMPM) (Hesthaven, 1998). This is an element based method that ensures less numerical dispersion and more accuracy than common schemes like the Finite Differences, Finite Element or Finite Volume methods. SMPM belongs to the family of the Spectral Methods, known for their accuracy, fast convergence and stability in different applications within Computational Fluid Dynamics (CFD). In particular, this method splits the BE into two operators (equation 3-4), a linear operator $L(u)$ for the diffusive term and a non-linear operator for the advective term $N(U)$ (Karniadakis et al., 1991; Peñaloza-Giraldo et al., 2015;

Preziosi-Ribero et al., 2016). Consequently, calculations are performed in two steps, the first one calculates the advective term via an explicit third order Adams-Bashforth scheme, and the second one uses an Euler implicit method for the linear part.

$$\frac{\partial \mathbf{u}}{\partial t} + \underbrace{\mathbf{u} \cdot \nabla \mathbf{u}}_{N(\mathbf{u})} = \underbrace{\nu_a \Delta \mathbf{u}}_{L(\mathbf{u})}, \quad (3-4)$$

On the top the numerical scheme's takes as boundary condition velocity signals gathered from an existing Large Eddy Simulation (LES) model (Lian et al., 2019) at the top of a cubical packed 0,04 *m* diameter sphere bed. Results from this model have been validated with existing literature, demonstrating close correlation of numerical and experimental models (Manes et al., 2009). These velocity signals propagate within the rectangular *x*, *z* domain. For the left and right boundary conditions, the domain is periodical. At the bottom, the boundary condition is a fixed vertical velocity. For the initial condition, the model has a zero *x* and *z* velocity in the entire domain. The combination of initial and boundary conditions is similar to existing complex models that perform LES simulations and have detailed meshes that represent packed spheres (Lian et al., 2019). Nonetheless, the equation used for the present model is less expensive computationally since its mesh is not as fine as the one needed for LES or DNS (Direct Numerical Simulation) models.

The proposed model spans 60 *cm* in the *x* direction and 16 *cm* in the *z* direction, emulating the LES model that generated the input data for the 2DBE model (Lian et al., 2019). The model is discretized in square subdomains of different sizes in the vertical direction (figure **3-2**) giving more spatial resolution to the top, where the majority of changes in flow are expected to happen. For the case of the horizontal subdomains, the discretization is equally spaced since flow is expected to have the same mean behavior in this direction. Each one of the points shown in figure **3-2** represents a node for the SMPM discretization scheme. The space between nodes is divided in turn into 6 spaces using the Gauss-Lobatto-Legendre points. Therefore, the minimum element size is 0,125 *cm* located at the top, and the maximum size is of 1,0 *cm* approximately.

The results from the model are compared with experimental results from Particle Image Velocimetry (PIV) (Roche et al., 2018) in uniform beds and numerical results from an Large Eddy Simulation performed for flow over and into a cubical packed bed spheres (Lian et al., 2019). Flow results are compared to understand how well the proposed model performs against a complex numerical model as the LES and against experimental situations under different bed configurations. Mean velocities in both axis and turbulent stresses over depth are compared, hence a comparison between a regular bed, both numerically and experimentally are explored to assess the behavior of our simplified model.

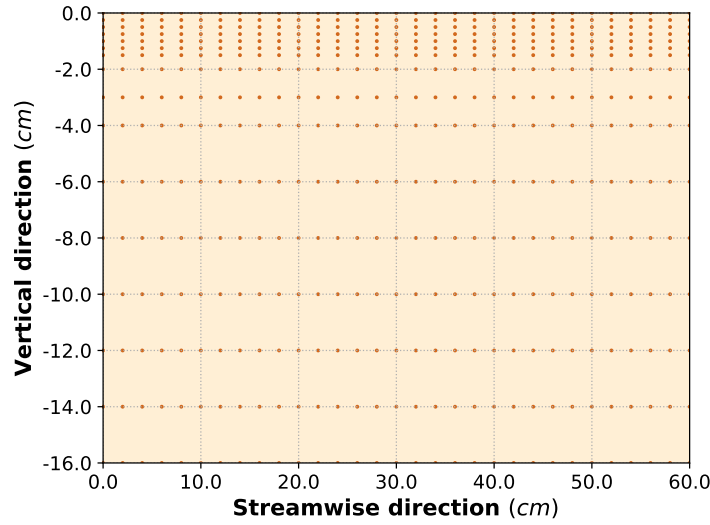


Figure 3-2: Node location for the problem (brown points). Note that the domain only corresponds to the river bed and does not include the free surface flow and that the coordinate $(x, z = 0)$ correspond to the separation between the stream and the bed. The computational domain is composed by 30 subdomains in the streamwise direction and 15 subdomains in the vertical direction. Subdomains have five points within them.

3.3. Results and Discussion

Our model simulated 100 s of time with time steps of $\Delta t = 0,03$ s to guarantee steady signals with non variant statistics. This section portrays the main findings of applying the SMPM to the 2DBE, while imposing changing boundary conditions from an LES model. As a first result, velocity signals were estimated using a probe in the middle of the domain, i.e. $x = 30$ cm, at different depths to describe flow behavior within the continuous porous medium (figures 3-3 and 3-4). The mean streamwise velocity decays with depth, as well as the variance of the signals (figure 3-3). In other words, signals appear to be closer to zero, flatter and less variable with the domain's depth. This decay is also the case for vertical velocity signals. However, for this case upwards (positive) and downwards (negative) velocities are present. This result is consistent, at least to some extent, with experimental results.

Most of the data probed for vertical velocity at $z = 0$ cm is positive, reflecting fluid ejections at that precise spot. Nevertheless, the vertical velocity signals below the shown point are negative, indicating fluid flow towards the bottom of the domain (figure 3-4). Furthermore, when comparing vertical and streamwise velocity signals, it is evident that their variability is different and it is likely that vertical velocity penetrates deeper into the domain than vertical velocity. Data, for both cases, is coherent since the signal lags before starting to fluctuate are almost the same either for vertical or streamwise velocity (orange, green and red lines in figures 3-3 and 3-4). Regarding horizontal velocities, the signals appear to be positive most of the time, going in the streamwise direction and decreasing with depth. In

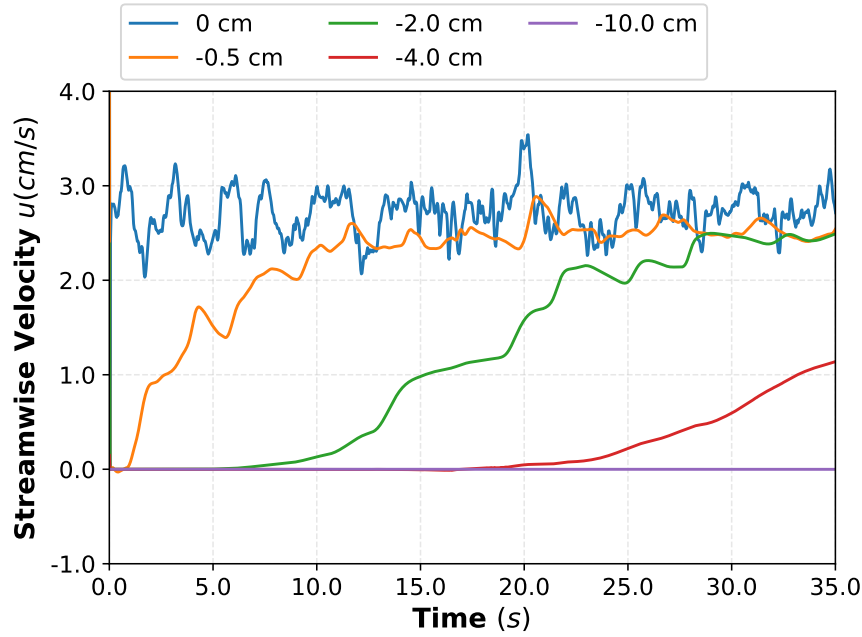


Figure 3-3: Streamwise velocity signals extracted at different depths at equal times. In blue: the input signal gathered from the LES model. In orange, green, red and purple: signals generated by the 2DBE model.

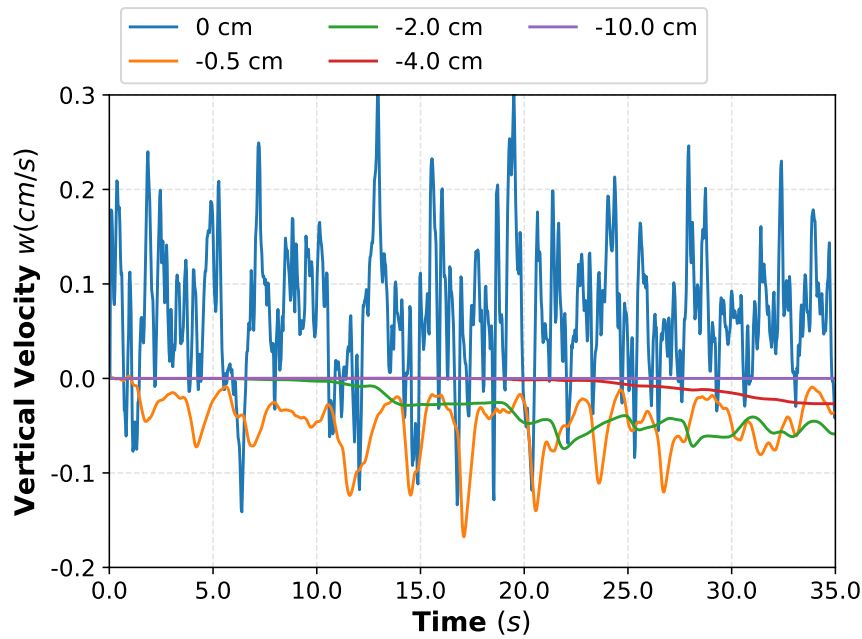


Figure 3-4: Vertical velocity signal extracted at different depths at equal times. In blue: the input signal gathered from the LES model. In orange, green, red and purple: signals generated by the 2DBE model.

brief, the velocity signals over the probe illustrate how the velocity evolves over time at each different depth. However, to assess the mean behavior with existing literature, it is necessary to compute time and space mean velocities and turbulent stresses (Pokrajac and Manes, 2009; Voermans et al., 2017; Roche et al., 2018).

Perhaps the most important outcome from the 2DBE is that the velocity is fully dissipated along the vertical domain. Namely, velocity at the bottom of the domain is equal to zero (figure **3-5-A**). This is particular, since the boundary condition for the bottom of the domain is a Neumann type boundary condition. However, this is possible, since the viscous term effects tend to dissipate the linear momentum, and if there was no bottom boundary, velocity would decrease until reaching a null value. The same results and reasoning is true for the vertical velocity, despite dissipating in a thinner space (figure **3-5-B**). Although flow properties decrease with depth, as recorded in the experiments (Voermans et al., 2017; Roche et al., 2018), our model underestimates the pore medium velocity by dissipating all of the velocity signals. To understand mean flow and try to find a reason why subsurficial velocity is zero, mean velocity and turbulent stresses are estimated.

The velocity results over the two dimensional domain are averaged over space and time, to obtain mean velocity profiles and mean turbulent stresses detected in the different signals (figures **3-5** and **3-6**). Additionally, results from experiments performed by Voermans et al. (2017) and Roche et al. (2018) are compared in their non-dimensional form with the ones obtained by the 2DBE model. Data is compared with existing literature whenever is possible since not all of the metrics and values are reported in both cited papers. Our results suggest that the 2DBE model mean streamwise velocity follows the one reported by experiments. For the case of Voermans et al. (2017), it has to be taken into account that these experiments were performed in heterogeneous beds, so results are expected to be different from 2DBE and Roche et al. (2018) (figure **3-5-B**). In any case, the comparison between homogeneous media models and observations in heterogeneous media allow this numerical experiment to take into account if the replacement of media properties by mean or average values are an efficient way to model a complex phenomenon.

The vertical velocity results from the 2DBE model are the second downside when comparing it to the experimental results (Roche et al., 2018). From the flume experiments, it is clear that vertical velocity has a high magnitude in the vicinity of the free surface flow and then it decreases monotonically until becoming almost negligible. Our model results suggest that vertical velocity has a considerably small value with respect to the maximum recorded streamwise velocity. The main reason why vertical velocity from the 2DBE model differs from experiments is the simplification made for the Burgers Equation. When assuming a linear pressure gradient within the bed, the effects of turbulent pressure variations are immediately neglected. This suggests that the vertical velocity, hence the inflow/outflow between a riverbed and a free surface flow are dominated by pressure gradients generated by bedforms, turbulent flow within pores, and pressure and form drags (Manes et al., 2011).

The hypothesis of vertical flow driven by pressure gradients is supported by the results of the streamwise turbulent stresses deviations (figure **3-6-A**). The magnitude, direction and values of these stresses are close when comparing experimental results and 2DBE model

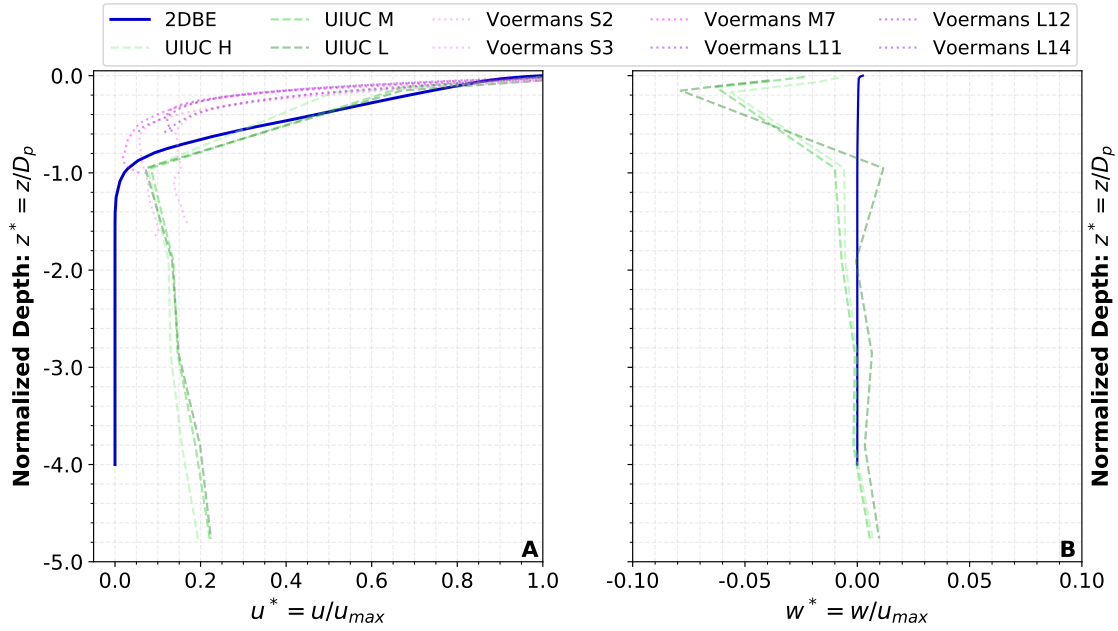


Figure 3-5: Normalized mean profiles: **A.** Streamwise velocity. **B.** Vertical velocity. For both of the plots, continuous lines indicate results from 2DBE.

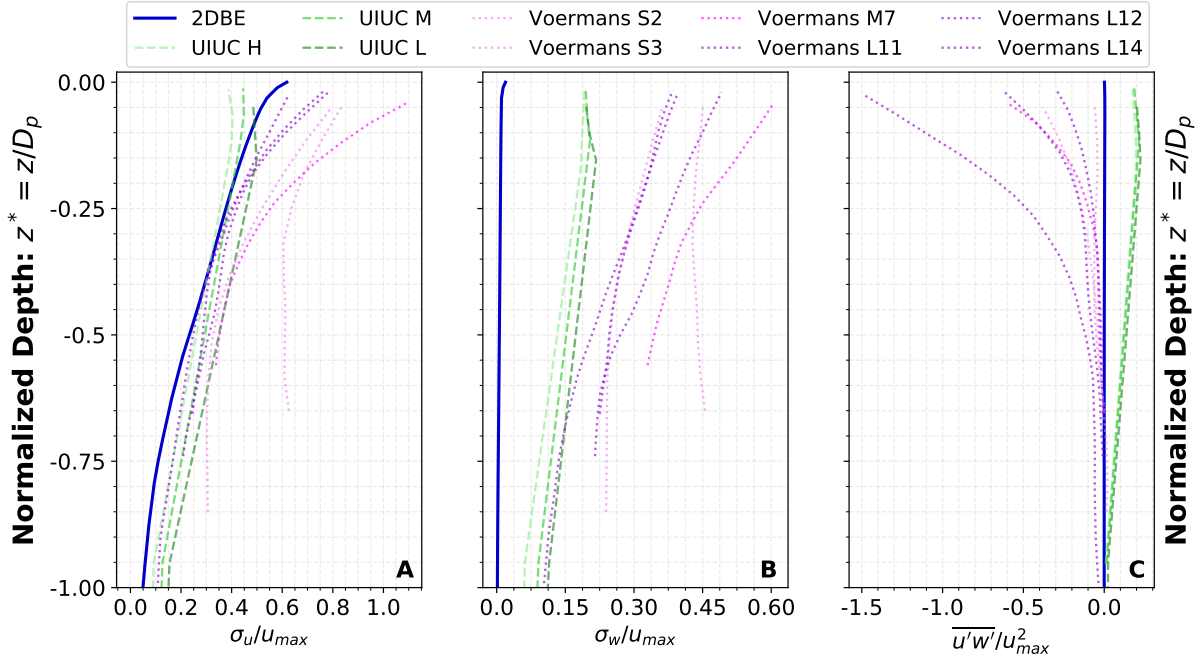


Figure 3-6: Normalized mean stresses profiles: **A.** streamwise turbulent stress, **B.** vertical turbulent stress and **C.** Reynolds stress. For all of the plots, continuous line indicate results from 2DBE.

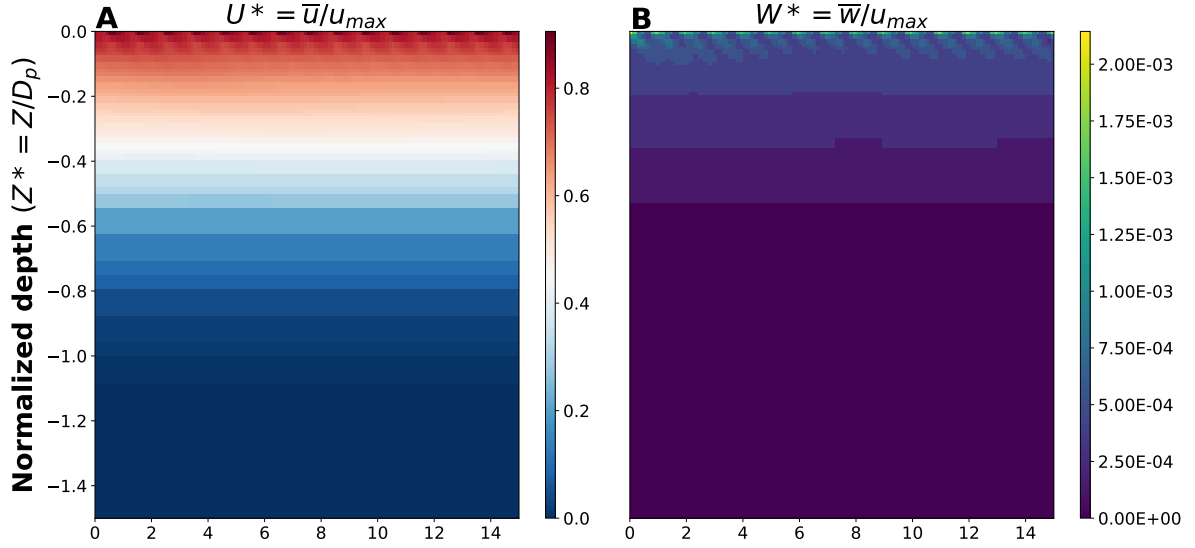


Figure 3-7: Mean nondimensional velocity heatmaps. **A.** Streamwise velocity. **B.** Vertical velocity. Domain is normalized by the mean particle diameter from the LES model (Lian et al., 2019).

outputs. In fact, most of the dotted curves from Voermans et al. (2017) group in packs according to the type of sediment used (see Voermans et al. (2017) for further reference), and the same can be observed from the experiments reported by Roche et al. (2018). For the case of vertical and Reynolds stresses, the results from 2DBE differ notably from the experiments' results. Indeed, our model predicts smaller values than the ones reported in the aforementioned experiments. One possible explanation for the missing that can be that HF is a three dimensional phenomenon and that the 2D simplification cut all of the influence of some turbulent stresses. Nonetheless, the chosen experiments report values from 2D observations and still report values for vertical and Reynolds stresses.

To get an idea of the flow behavior in space and its coherence and stability, different heat maps are presented to show the main variations of flow properties within the analyzed domain (figures 3-7 and 3-8). Results are presented in their non dimensional form to understand the way it appears to be driven by the mean diameter of the particles from the LES model (Lian et al., 2019). Therefore, a value of 1 in the z^* coordinate indicates one particle diameter. Results show a mean behavior over the whole analyzed domain and are plotted only over a vertical span of 1,5 sphere diameters, since no mo relevant changes happen in deeper coordinates. It is possible to identify the LES model effects at the top of the domain, where vertical velocities tend to fluctuate and show visible differences (figure 3-5). However, these strong velocity gradients are immediately smoothed out by the effects of advection and diffusion in the 2DBE. These effects are also present in the vertical turbulent stresses and the Reynolds stresses, since they depend also on the vertical velocity signals (figures 3-6-B and 3-6-C). Summing up, our results suggest consistency with flow properties behavior, now this behavior is to be assessed along different experimental results to draw significant conclusions about 2DBE.

In a nutshell, 2DBE model was expected to perform better in the vertical direction. In fact, for the plots of vertical and Reynolds stresses, the 2DBE model plots were expected to fall somewhere near the green dashed lines that are nicely grouped in a single sector showing a strong correlation between maximum velocity and turbulent stresses (Roche et al., 2018). For the case of the dotted lines, stresses seem to be located with no grouping at all in the different plots (figures **3-6A**, **B** and **C**). However, when looking closely, these curves are grouped by the sediment size (S for “small sediment”, M for medium sediment size and L for large sediment size). Once again the reader is encouraged to check Voermans et al. (2017)). This indicates that in natural media, contrary to ideal porous media studied in this research work, the grain size distribution is a key driver of turbulence penetration within porous media in the HZ. In brief, the 2DBE model is able to model to a certain degree of precision the mean features of streamwise velocity, lacking of precision or utility in the vertical direction due to the misrepresentation of pressure terms in the Burgers equation.

3.4. Conclusions

A 2D numerical model based on the Burgers’ Equation was built to assess HF in an idealized granular media, emulating an existing numerical LES experiment (Lian et al., 2019). Our model simulated only the porous bed, taking as top boundary condition the velocities generated by the aforementioned model. The Spectral Multi-Domain Penalty Method was used to minimize numerical diffusion and spurious signals presence, assuming in the meantime stability and precision with a third order Adams-Bashforth explicit scheme, an explicit solver for the advective part and an implicit method for the diffusive part. The main idea was to solve mean flow features without the need of complex models with extensive computational and time usage.

The 2DBE model results were assessed with data from flume experiments in both homogeneous and heterogeneous media. This comparison showed that the 2DBE model is not precise to model all of the features of HF in detail. On the one hand, it performs well for streamwise velocity and horizontal turbulence stresses, showing agreement with both experiments that was compared with. On the other hand, results from vertical velocity and vertical stresses were not close to the values reported in literature because of the simplifications that imply the use of the Burgers’ Equation for modeling Hyporheic Flow. This implies that pressure and its turbulent fluctuations are important and drive vertical flows, at least in the cases of flume experiments analyzed in this chapter.

Further use of the Burgers’ Equation to model Hyporheic Flow is discouraged, since the addition of drag terms to account for flow attenuation is not based physically entirely and can lead to violations of conservation of physical quantities such as mass. In addition, the addition of more terms does not solve the lack of pressure gradients within the modeled domain. Consequently, it is important to find an expression based on (i) mass and momentum conservation, (ii) taking into account pressure fields within the flow domain, (iii) momentum source/sink terms can be added apart from the pressure term to account for the effects of porous media on the mean flow. The following chapter will explore the use of a commercial

NSE solver using a Finite Volume Scheme and taking into account the whole flow, i.e. free surface flow and groundwater flow.

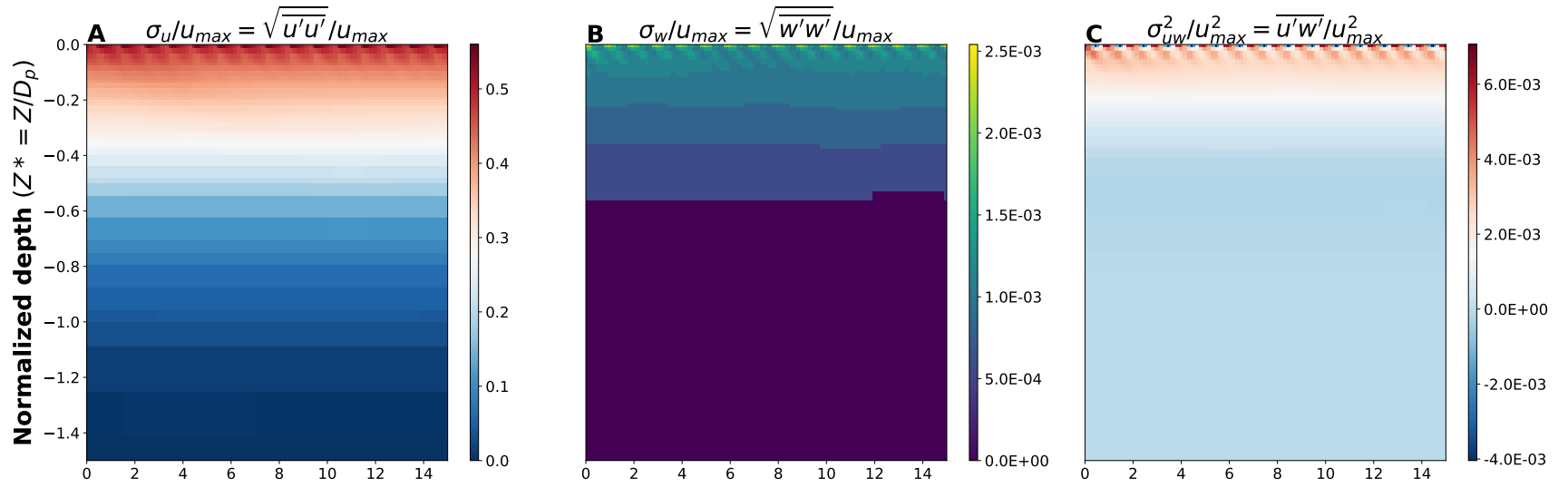


Figure 3-8: Mean turbulent stresses over the entire domain. Stresses are normalized using the maximum streamwise velocity recorded by the 2DBE model. **A.** Streamwise turbulence intensity. **B.** Vertical turbulence intensity. **C.** Reynolds stress

4 Coupling Free Surface Flow over Permeable Porous Beds

Since the Burgers' equation model was not able to represent properly the hydrodynamics of HZ, a model using the full Navier-Stokes Equations is introduced in this chapter to evaluate its performance against flume experiments. The apparent viscosity coefficient was also used for this case. However, source/sink terms were added to model the heterogeneous media as external forces exerted to the flow within the porous domain. Here, the Finite Volumes Method is used as the numerical scheme via the OpenFOAM package. Our results show a more realistic behavior than the ones obtained in chapter 3. The work presented in this chapter is based on a working paper by Saavedra-Cifuentes and Preziosi-Ribero.

A numerical model is implemented for the simulation of a free-surface flow over a permeable bed assuming a continuous computational domain containing both regions. Pressure and velocity fluctuations coming from the turbulent surface flow are effectively considered in the model by representing the porous river bed as an additional diffusive term in the momentum conservation equation, similar to the common strategy of adapting drag terms for this purpose. Two types of simulations were executed: 1) a cavity-type simulation in order to compare the results from the model with the additional diffusive term and the model that adopts the drag terms. 2) a channel flow simulation representing a flume experiment over a permeable bed with regular bed geometry and adapting a scalar transport equation simulating a dye tracer that penetrates the porous bed. For the first case, results suggest that the overall behavior of both models are similar but the calculated velocity and pressure fields vary on the interface between the free surface flow and the represented porous media. For the second case, differences are more notable when assessing the flow structure in-between dunes. The transport simulation of the dyed surface water from both drag and diffusive models are compared with the physical model. Results suggest that both approaches are able to represent the interaction between the turbulent surface water flow and the laminar groundwater flow inside a porous bed, but the proposed model helps to better represent free surface flow features regardless of the initial condition use in the simulation.

4.1. Introduction

Hyporheic Flow (HF) is a key driver for the ecological equilibrium in river corridors and the environmental stability of fluvial aquatic ecosystems Kalbus et al. (2006); Boano et al. (2014). Mixing of surface water and groundwater in this zone provides exchanges of mass, momentum and energy, which are basic inputs for life development (Boano et al. (2014); Cardenas (2015) and references therein). Moreover, this phenomenon is present at a wide range of length scales that span from the pore-size to several meters, and time scales that vary from seconds to hours or even days, i.e. defining the limits of the influence of HF in river corridors remains an open challenge for the scientific community (Bencala, 2000; Boano et al., 2014; Cardenas, 2015). However, knowledge of the flow patterns and its drivers within the Hyporheic Zone (HZ) is a topic of interest for ecological purposes, nutrient and contaminant transport, river restoration and even Water Resource Management.

Current HF models divide flow into two separate domains that communicate through boundary conditions, i.e., a zone of turbulent free flow and a zone of laminar flow where Darcy law holds (Discacciati et al., 2002; Boano et al., 2014; Cardenas, 2015). Therefore, the exchange of mass, momentum and energy is treated as a scalar transport problem with expressions such as the Advection Dispersion Equation (ADE) of any solute of interest Clark (2009). For the representation of the porous media, two approaches are common: i) consider the domain as a continuum or ii) consider the geometry of porespace individually. For the specific case of hydrodynamics, one dimensional models of vertical velocity attenuation are used to explore the dissipation of turbulence in a continuous bed in either one, two or three dimensions. More complex models consider averaging the Navier-Stokes Equations (NSE) in spatial scales to obtain averaged expressions that take into account the presence of obstacles as drag terms (Breugem et al., 2006). However, the modeling techniques and physical processes vary across scales, identifying different drivers for this phenomenon at different scales (figure 2-6).

Nonetheless, transport in rivers is always turbulent and highly advective Elliott and Brooks (1997b). As a consequence, the velocity field (i.e., the hydrodynamics) has to be first defined in order to characterize these exchanges between surface and groundwater. Moreover, current approaches neglect the presence of turbulent structures inside the porous bed following Darcy's law. However, flow in a porous media is not always laminar Bear (1975); Barr (2001) and flow near a permeable wall is ruled by turbulent structures, which are a source of the momentum exchanges between the channel and the permeable bed (Breugem et al., 2006; Ghisalberti, 2009; Manes et al., 2011). In addition, water exchange within the riverbed has a convective driver which implies that vertical velocity gradients are important Manes et al. (2012); Ghisalberti (2009), leading to the rejection of any NS equations reduction where the vertical direction is not considered. Therefore, a conciliation between these two different flow regimes (i.e., free surface and porous media flow) is necessary: the free surface flow where the velocity field is clearly distorted by the turbulence effects, and the porous region usually assumed as a region of laminar flow (since Darcy's Law is considered valid).

The main goal of this section is to assess a model that includes both free surface and porous media domains to: i) compare it with the existent models that also meet these assumptions, and ii) compare with experimental results to explore its validity in a typical dune scale. To

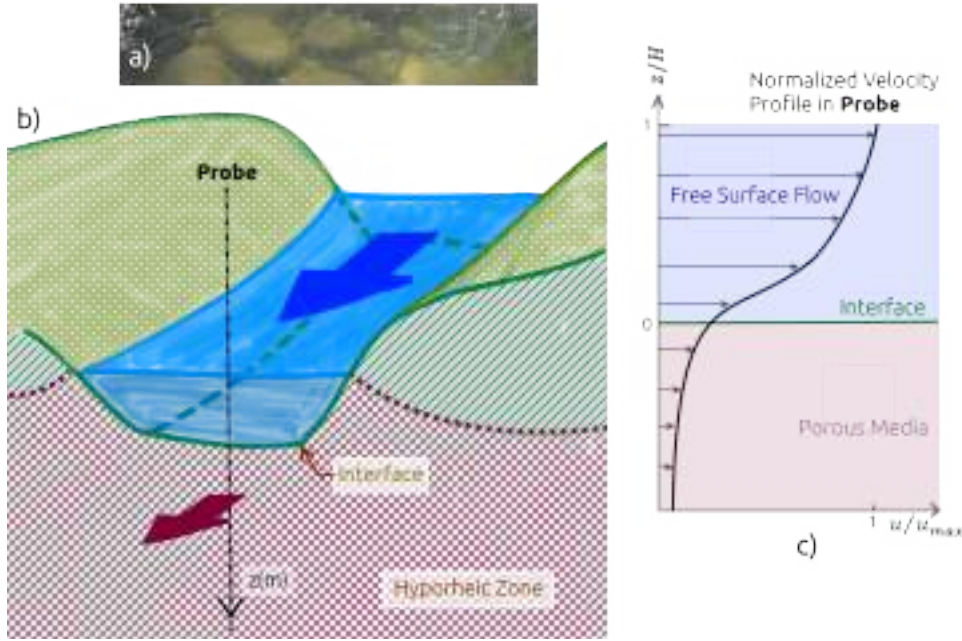


Figure 4-1: Riverbed in Guali River - Colombia (a), schematics (b) and velocity profile (c) for a free surface flow over a permeable bed. The velocity at the interface is not zero but it is damped proportionally to depth.

achieve this goal, a previously built open source code (Weller et al., 1998) is used and modified to include different parameters that can represent the flow resistance within the porous media and flow without restrictions in the free stream part. Our model's main contribution is coupling two domains that were usually considered as separate media, or sometimes modeled with high detail in packed geometries that are not representative of granular media (Lian et al., 2019). The interface between the free surface flow and the permeable bed is defined by a nondeformable surface, i.e, sediment is assumed immobile. In addition, the position of this interface is often clearly defined, as shown in Figure 4-1.

By implementing this model, novel information is gained regarding the transition between turbulent flow in a free surface stream and a defined porous region. This approach allows us to group all of the physical processes present in the macro scale and replace them within the Navier-Stokes equations as drag coefficients or viscous forces that hinder flow due to the resistance generated by the grains and structures inside the porous media. The assessment takes into account different flow conditions and different resistance coefficients that model different types of porous media. This paper is divided in four sections. First, the proposed model is presented in detail; then in the Benchmark Case comparison, our hydrodynamics results are compared with the ones obtained in previous numerical models. From that point, our model results are used to run a solute transport simulation and check its validity in a stationary case. Finally, the results are discussed in detail and conclusions are drawn from the proposed approach with its advantages and downsides.

4.2. Proposed Model

The numerical model that simulates the interaction of free surface water and groundwater in riverbeds is proposed by adopting the two-dimensional incompressible NSE for momentum and mass conservation in a continuous computational domain that contains both free-surface and permeable bed subdomains. The pressure gradient term is conserved, contrary to previous approaches (Higashino and Stefan, 2008; Preziosi-Ribero et al., 2016); therefore the pressure field is calculated from the governing equations. In addition, the mean turbulent effects are evaluated by adopting a standard two variable turbulence model ($\kappa - \epsilon$ model), that is commonly used in different numerical schemes. This model implements a higher viscous diffusion coefficient $\hat{\nu}$ in the NS equations and it is adopted for characterizing the permeable region (Equation 4-1). As a consequence, momentum losses inside the porous media are modeled as a predominantly viscous diffusion process. Here, u stands for the velocity vector field, P for the pressure scalar field and x for the spatial coordinates in tensorial notation with sub-indexes i and j representing the different dimensions.

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \hat{\nu} \frac{\partial}{\partial x_j} \frac{\partial u_i}{\partial x_j} \quad (4-1)$$

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (4-2)$$

The diffusion coefficient term $\hat{\nu}$ in Equation 4-1 takes two different values: i) for the surface flow, it will correspond to the kinematic viscosity of the fluid, in this case assumed constant (with $\nu_m = 10^{-6} m^2/s$ as a typical value); and ii) for the porous region within the domain, this viscous diffusion coefficient takes a greater value in order to restrict the velocity field. Therefore, at the porous region viscous diffusion coefficient is equal to an apparent viscosity ν_{ap} 4-3, some orders of magnitude higher than the one of water in the free surface flow.

$$\nu_{ap} = \frac{\phi g d^2}{32K} = 5,625 \nu_m \left(\frac{d}{d_s e} \right)^2 \quad (4-3)$$

The term ν_{ap} is a diffusion coefficient set to emulate the difficulty for the water to flow through an obstructed medium as a porous matrix. The relationship between this parameter and the macroscopic parameters that represent the porous medium used by Higashino and Stefan (2008); Peñaloza-Giraldo et al. (2015) is obtained by considering two different laminar flow models -Equation 4-3- where ϕ , e , K and g represent the porosity, void ratio, hydraulic conductivity and gravity acceleration, respectively; d and d_s represent the void and solid particles mean sizes. Porous media is typically represented in two ways: as a capillar tube model and the hydraulic radius models, from which the Kozeny-Carman equation is deduced

Bear (1975). Therefore, apparent viscosity could be calculated from two ratios measured from bed properties: the voids ratio, and the ratio between pore size and mean particle size. Equation 4-3 could be used to get an estimation of the apparent viscosity, however, different orders of magnitude are evaluated in Section 4.4 to assess whether this expression yields a useful estimation from the modeling perspective.

To compare our model's results with other approaches, a second model that includes drag terms within the 2D-NSE is also implemented. This model is similar to the ones proposed by Hsu et al. (2002) and del Jesus et al. (2012) for waves and porous coastal interaction. In these models, the authors solved for the hydrodynamics inside the porous subdomain by a Volume Averaged Reynolds Averaged Navier-Stokes (VARANS) set of equations, which characterize the porous media by its porosity and a set of drag coefficients, called Forchheimer's coefficients (A and B in equations 4-4 and 4-5) Whitaker (1996)). Additional information about current modeling approaches for GW-SW interactions is available in this paper's supplementary information.

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \nu \frac{\partial}{\partial x_j} \frac{\partial u_i}{\partial x_j} + A_d u_i + B_d |u| u_i \quad (4-4)$$

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (4-5)$$

4.3. Benchmark Case Comparison

To compare the results between the Drag-NS model and the proposed apparent viscosity model, a cavity flow case with two different flow regions is proposed. The configuration for the porous region used in this experiment consisted of a 1×1 m box and no-slip boundary conditions for every side except the top boundary where a 0.1 m/s velocity was set (figure 4-2). A Reynolds number ($Re = uL/\nu$) is defined with the box depth and velocity at top boundary as characteristic length (L) and velocity (u), respectively. As viscosity (ν) changes in both regions, two different Reynolds numbers exist in the computational domain. Therefore, we propose a Reynolds' number ratio (RNR) as the relation between the free surface flow and the permeable region Reynolds numbers. Particularly for this case, RNR becomes a relation between viscosities.

First, our model was evaluated with a RNR of 1000 by setting the viscosity to 10^{-3} m²/s for the upper region and 10^0 m²/s for the porous region. When a steady solution of this problem was reached, the same case was set for the Drag-NS model and A_d and B_d were calibrated to get the most similar solution in comparison with the previously described case. This calibration process was performed by adopting the Dynamically Dimensioned Search (DDS) algorithm (Tolson and Shoemaker, 2007) for minimizing a root mean-squared error computation with the software OSTRICH Matott (2017). For this particular RNR , it was

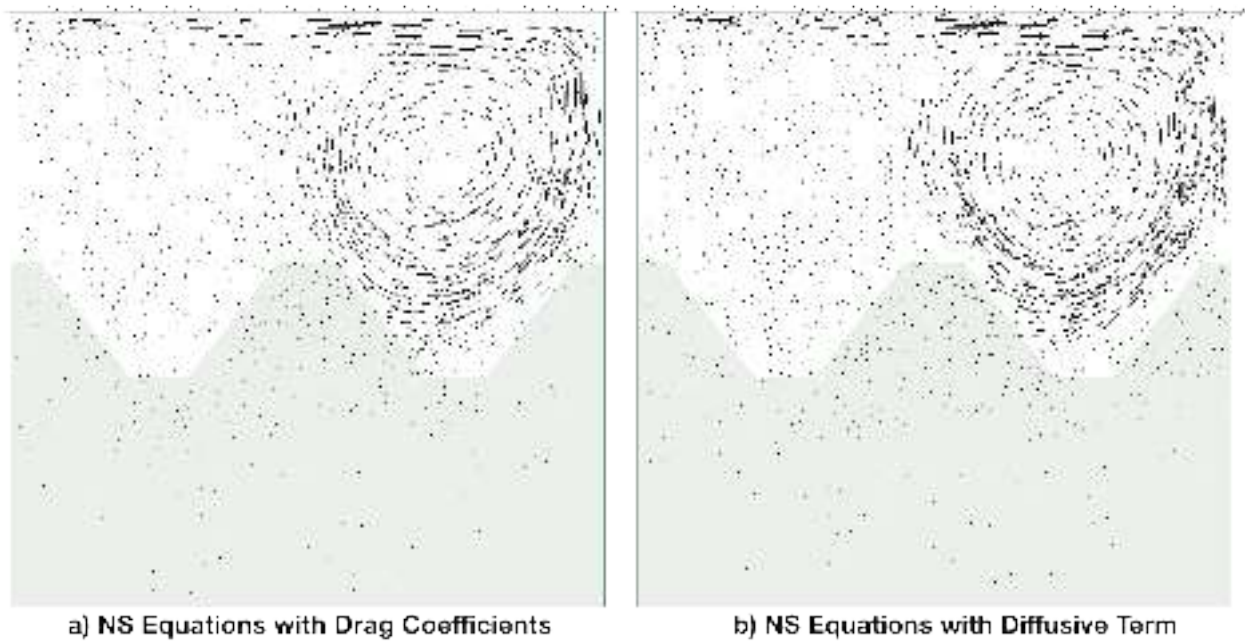


Figure 4-2: Velocity vector map of the results obtained when implementing the Drag-NS model (a) to a cavity type experiment and its equivalent proposed model (b)

found that the optimal values of A_d and B_d to adjust the proposed model solution where $0,68 \text{ s}^{-1}$ and $48,4 \text{ m}^{-1}$, respectively.

The effect of the cavity with the trapezoidal obstacle for the formation of the main eddy is evidenced in numerical and physical models of this same case Botella and Peyret (1998); Erturk et al. (2005). It is also present in our model (figure 4-2), fostering the formation of the main eddy in the part where viscosity is lower. Although the obstacle acts as a permeable region where flow still can be developed, it does affect the length scale constraining the eddy development. Some differences can be identified when the velocity and pressure fields are compared, albeit the similarity of the overall behavior of both velocity fields.

Figure 4-3-a shows the azimuth absolute difference between both obtained velocity fields: it ranges from 0° when velocity vectors point the same direction to 180° when they are totally opposed. The greatest discordance of velocity directions is located at the trough of the dune: where the solution implementing the proposed model predicts flow downwards in the vertical direction, the solution with drag coefficients supposes a flux upwards due to a second smaller eddy. Velocity differences in magnitude are shown likewise in figure 4-3-b: blue boxes represent points where a higher velocity was predicted from the drag coefficients while green diamonds represent higher velocities found with the proposed model. For this case, the more evident disagreement between the two models occur immediately over the interface where the main eddy on the free-surface region contacts the permeable media. This disagreement is also evident when the pressure fields are compared. In Figure 4-3-b, the pressure field from the Drag-NS model is subtracted from the proposed model's pressure

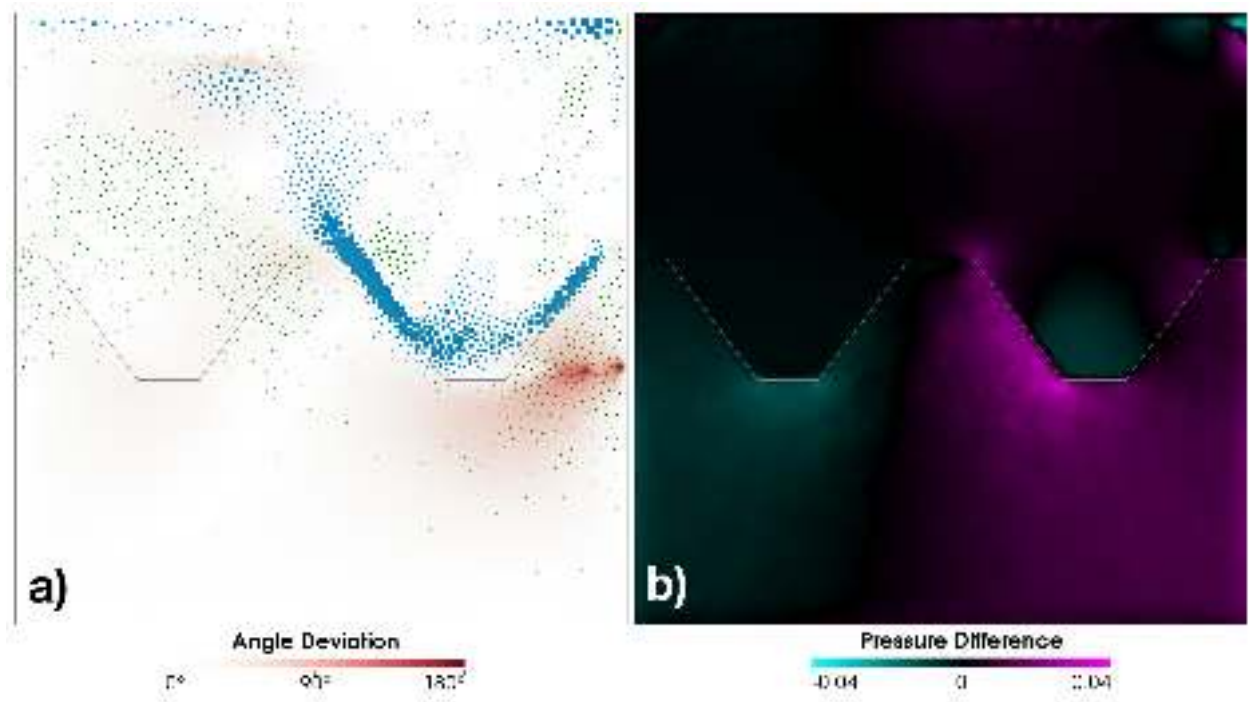


Figure 4-3: Angle deviation and magnitude discordance (a) and pressure field difference (b) of the velocity vectors calculated from the proposed model and the equivalent Drag-NS model

field: lower and higher pressures given by the proposed model compared to the drag model are represented by purple and green dots respectively. It is interesting that the pressure field near the interface, where the velocity fields disagree, also differs one from the other, i.e., the pressure field obtained with the proposed model is higher than the one resulting from the drag terms.

At this point, it has been shown that there are differences in the results obtained from both models. However, the lack of experimental data hinders the assessment of which model better represents the physical behavior of the SW-GW interaction. Thus, a comparison with real data is described in Section 4.4.

4.4. Laboratory Experiment and Validation

Our model was compared to the dye injection flume experiments from (Fox et al., 2014). The flume setup consisted in a surface flow over a poor graded sand. For our case, a scalar transport equation was solved in steady state for the calculated velocity field and its results were used to identify the dye penetration patterns inside the permeable bed. Therefore, identifying the area where the turbulent flow would have an incidence inside the porous media flow, i.e. the hyporheic zone of the model. Since velocity or pressure measurements were not performed in every point of the experimental setup, special attention was given to

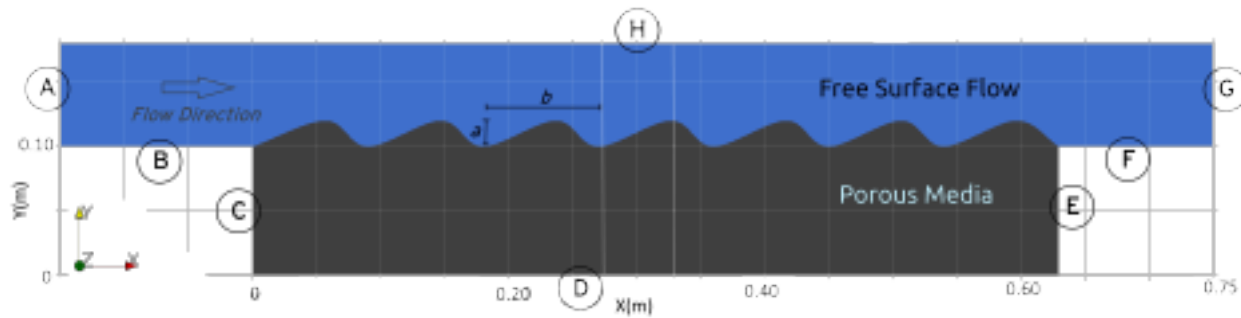


Figure 4-4: Computational domain for simulating flow over dune-shaped bed forms from the laboratory setup

the dye intrusion visualization.

4.4.1. Computational Domain

The simulation was performed in a two-dimensional domain comprised by a free surface flow region over a permeable porous region, shown in Figure 4-4. Encircled letters identify each boundary of the computational domain which follow the following boundary conditions for velocity: a no-slip condition in faces B, C, D, E and F; a constant flow inlet at face A; a slip condition on face H equal to the reported velocity in the laboratory setup ($0,123 \text{ m s}^{-1}$) and a zero-gradient Neumann condition on face G. These conditions were imposed for all faces for the pressure field, except for the outlet face G where a Dirichlet condition was given ($P = 0$). The laboratory installment was longer than the computational domain defined in this work, however, after some simulations it was clear that for the presented geometry, the effects of the boundary conditions were not visible on the hydrodynamics on the middle dunes which were chosen for all the following analysis. The dunes geometry was estimated from the flume photographs reported in Fox et al. (2014). Those dimensions are indicated as a and b in Figure 4-4 and they are equal to $0,15 \text{ m}$ and $0,02 \text{ m}$ respectively. The spatial discretization was built on GMSH Geuzaine and Remacle (2009) and a mesh independence test was performed as well.

4.4.2. Velocity Fields and Free Surface Flow behaviour

The simulation was performed representing the porous media with different orders of magnitude of apparent viscosity ($\nu_{ap} = [10^{-2}, 10^0] \text{ m}^2/\text{s}$) and drag coefficients until a steady-state solution was reached in every case. Then, velocity profiles (Figure 4-5) were extracted at the top and bottom of the middle dune at the dotted vertical lines appearing in Figure 4-4. There is an order of magnitude for both the apparent viscosity and the drag coefficients from which the calculated resembles more to the flow behavior over a solid permeable bottom. For the apparent viscosity case, this limit order of magnitude is $O(\nu) = 10^{-2} \text{ m}^2/\text{s}$.

Our results suggest that the velocity fields calculated are similar for both the Drag-NS and

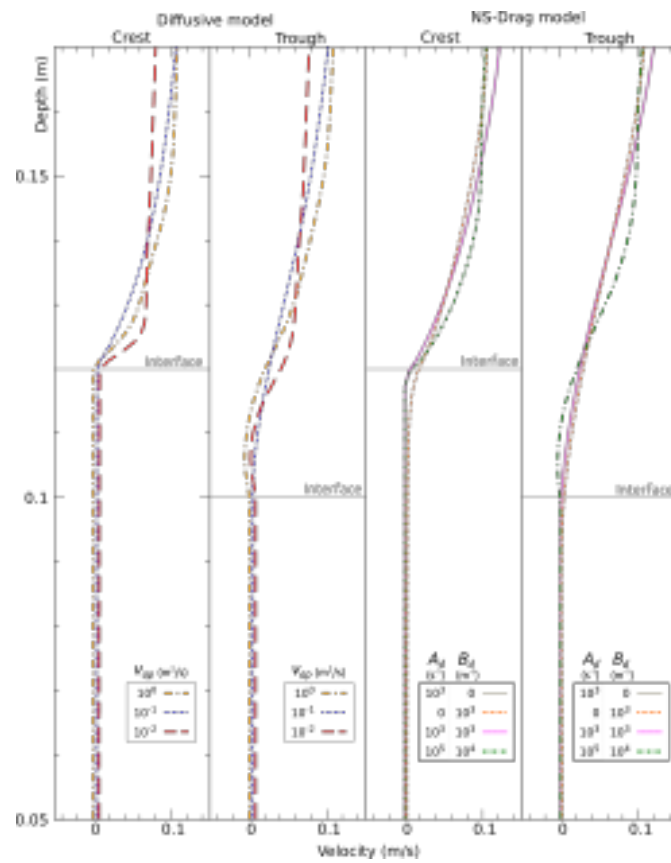


Figure 4-5: Velocity profiles for different values of apparent viscosity and drag coefficients

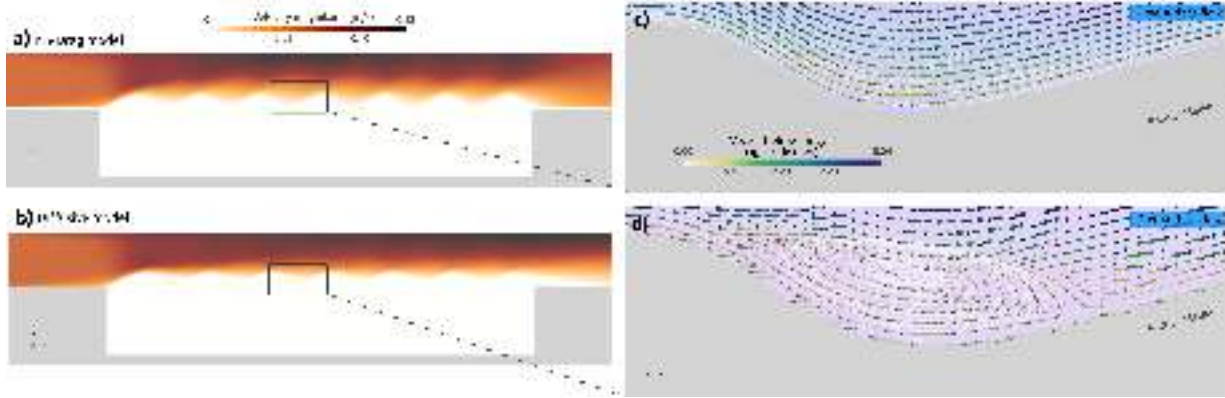


Figure 4-6: Velocity field calculated for a porous region represented by (a) $\nu_{ap} = 1$ and (c) $A_d = 10^5$, $B_d = 10^5$. Detailed windows for each case are shown in (b) and (d) respectively

the apparent viscosity models, except at the dunes' troughs where negative velocities develop near the sediment-water interface (marked by a horizontal line). This is clearer in Figure 4-6-b and 4-6-d where the detail of the velocity field in that particular region is examined for the apparent viscosity model and for the Drag-NS model, respectively. The former is able to represent the recirculation flow similar to the one obtained by Cardenas and Wilson (2007a), thus, conciliating the existence of a permeable bed under the interface and at the same time leading to a similar structure of the free surface flow. The model that used the Forcheimer's drag terms fails in forming this pattern, despite the high values used for the A and B coefficients tried for this purpose. This particular case is assessed in section 4.5.

For the free surface flow region, Reynolds' number was defined with the mean depth and top boundary velocity as characteristic length and velocity respectively. On the other hand, the permeable region Reynolds' number was calculated with the same velocity and with the dune length. It was found that when the apparent viscosity's order of magnitude exceeds $O(10^2)$, Reynolds' number on the permeable region exceeds a value of 1,0, which agrees with the point where the simulation behaves more of a free surface over a solid permeable bed, rather than a two-phase non-mixing fluids system. Furthermore, the RNR varied from 10^6 to 10^4 , which are higher values than those used in section 4.3.

4.4.3. Scalar Transport Simulation

For the set values of apparent viscosity and drag coefficients, a scalar transport simulation was executed in order to qualitatively compare the photographs reported by Fox et al. (2014) of dye penetration from the free surface flow inside the sand dunes for a neutral condition, i.e., no inlets nor outlets were allowed from the bottom of the computational domain. To achieve this comparison, a standard ADE was implemented using the velocity field obtained from the simulations and standard ink diffusion coefficient. The best fitted penetration patterns testing the proposed model and the Drag-NS approach are reported in figure 4-7-a and

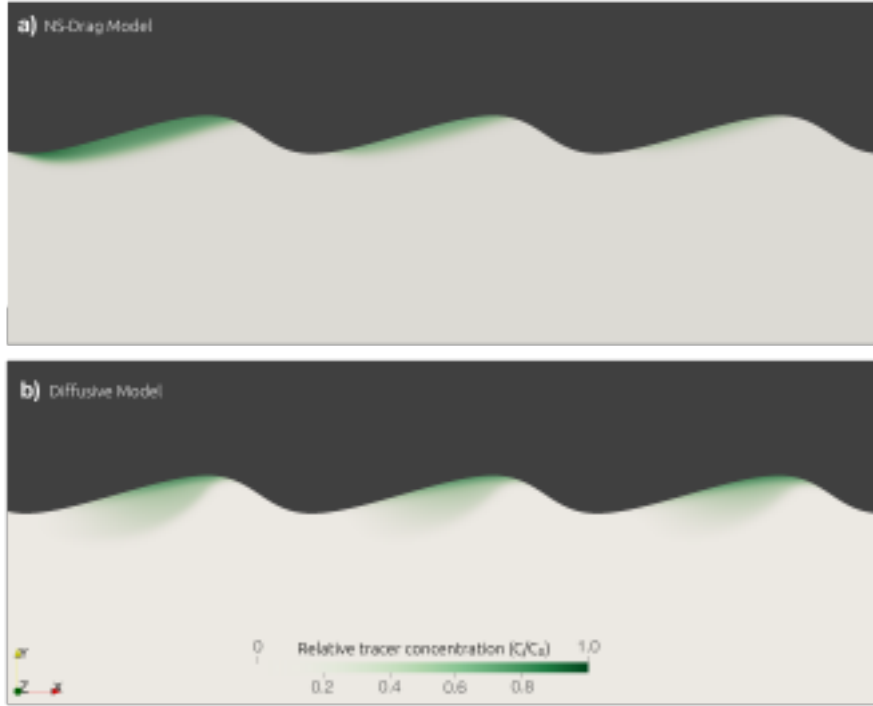


Figure 4-7: Scalar transport simulation results for dye penetration into porous dunes represented by (a) $\nu_{ap} = 1$ and (b) $A_d = 10^2$, $B_d = 10^2$

4-7-b, respectively. When comparing this results to the laboratory evidence, the pattern obtained from the Drag-NS approach is more alike to the one obtained using the apparent viscosity since the curvature of the dye intrusion under the dune top is clearer, contrary to the results from using the apparent viscosity where dye is already invading the downstream face of the dunes, which is not stained at any moment in the experiment.

However, our results are not able to represent the outcome of the physical experiment in detail. The color map obtained from the dye penetration in the numerical model follows a more regular pattern than the one exhibited in the experiments for all of the performed numerical simulations. The results presented in the physical experiments (Fox et al., 2014) are photographs where concentration values are not available. Therefore, our results are just comparable with the experiments for their shape and maximum dye penetration in the porous media. This limitation makes the calibration process between numerical results and experiments an open challenge. Nevertheless, the dye penetration experiments were performed in a porous media partially clogged by fine sediments, while our model considers homogeneous media with no spatial variations.

4.5. Discussion

Results from the Drag-NSE model do not lead to the same results than our apparent viscosity model. This is particularly evident in the sediment-water interface where calculated pressure

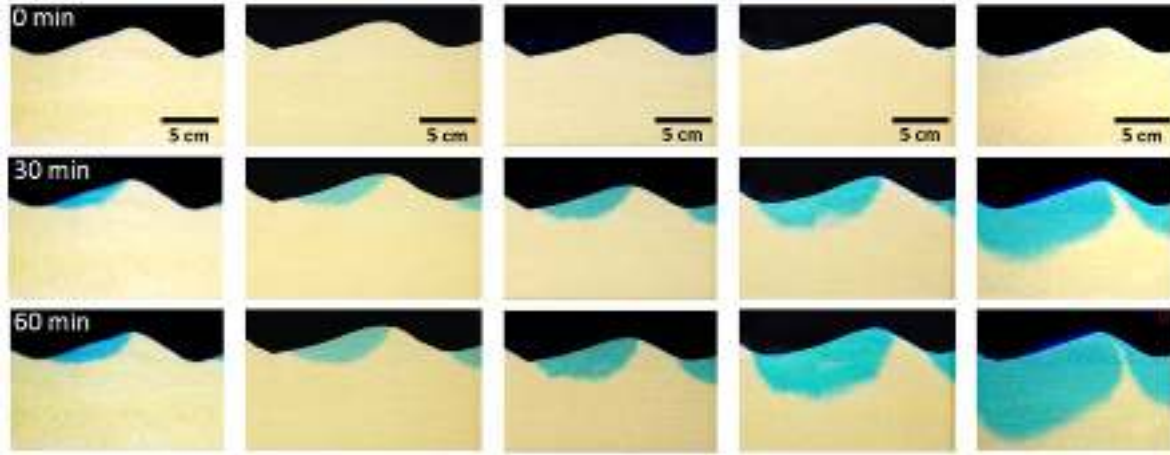


Figure 4-8: Dye injections performed by Fox et al. (2014). Patterns from neutral case are compared with numerical experiment from figure 4-7

and velocity fields differ the most. However, for the most part of the domain simulated in section 4.3, the overall flow behavior is similar between both of the models. Furthermore, modifying the parameters in the Drag-NS model used in the experiment on Section 4.4 never reached the flow behavior obtained from the proposed diffusive model. To assess the differences between the results observed when implementing Equation 4-4 and Equation 4-1, it is useful to identify that these two equations appear to be equivalent when:

$$\hat{\nu} \frac{\partial}{\partial x_j} \frac{\partial u_i}{\partial x_j} = A_d u_i + B_d |u| u_i \quad (4-6)$$

In order to compare both models, an assumption is made about the advective and pressure terms, albeit non-negligible, they are less important than the others. This is true when flow velocity decreases near the sediment-water interface, the diffusive term on Eqn. 4-1 and the drag terms on Eqn. 4-4 become more important on each of the obtained solutions. Therefore, the comparison given in Eqn. 4-7 is proposed.

$$\begin{aligned} \partial u_i / \partial t &= \hat{\nu} \frac{\partial}{\partial x_j} \frac{\partial u_i}{\partial x_j} \quad (a) \\ \partial u_i / \partial t &= A_d u_i + B_d |u| u_i \quad (b) \end{aligned} \quad (4-7)$$

Solution for Eq. 4-7(b) is restricted to the initial condition of u while Eq. 4-7(a) requires both initial condition and boundary conditions around x_i . In the case of no-slip boundary conditions and an initial condition whose second derivative exists, the solution on a time $t + \Delta t$ from the diffusion equation (i.e., Eq. 4-7(a)) is met choosing the appropriate constant values A_d and B_d , however, this is restricted by the concavity matching the initial condition function's sign, which can be broken down to two specific cases: i) For the diffusive model

(and with ν positive) a concave downward function $u_i|_t$ yields $u_i|_t > u_i|_{t+\Delta t}$ until reaching a steady state, whereas, ii) for the drag-NS models (also with A_d and B_d positive) a positive function $u_i|_t$ yields $u_i|_t > u_i|_{t+\Delta t}$ until reaching a steady state. This is the case for the results obtained in the first experiment where no-slip boundary conditions are imposed at most of the faces, no inflow or outflows are considered and a fairly good approximation is obtained by calibrating for A_d and B_d .

The second case experiment has different boundary condition values and mass inflows and outflows, thus non-homogeneous non-zero boundary conditions governed the problem and the steady state reached by the diffusive model differed significantly from the solution given by the drag-NS model. In addition, the velocity field was predominantly oriented towards the positive x axis, different of the first case where velocity vectors were found in every possible direction. Only positive values on the initial condition causes $u_i|_t > u_i|_{t+\Delta t}$, however concavities both upwards and downward were present, thus, violating the rules given for the Drag-NS model matching the proposed model. To corroborate this, the initial condition was changed for the Drag-NS model in this experiment adopting the steady state solution from the proposed diffusive model, encountering a new steady state solution that was actually similar to the diffusive one.

Regarding the influence of dynamic pressures on the solution, a volume of fluid (VOF) simulation was initially proposed for the numerical representation of this case Saavedra-Cifuentes (2017). but it was found unnecessary to calculate the water surface position since it was relatively constant during the experiment. It is to note that a smooth water surface is not enough reason to believe that a hydrostatic pressure distribution is appropriate to represent this phenomenon since flow is almost never parallel to the bed forms and curvature of flow paths is developed, thus, dynamic pressure had to be taken into account.

4.6. Conclusions

Novel numerical simulations of a complete domain containing both free surface flow and porous permeable regions were performed by coupling surface flow and permeable regions via the diffusive term in the Navier-Stokes equations for momentum conservation. The pressure field was considered variable and non-linear in the model, adopting an apparent viscosity as a higher diffusion coefficient for the momentum transfer inside a porous region and comparing with other approaches regarding the mathematical representation of porous media with some constant drag parameters. A first experiment similar to a cavity flow problem was set with no mass exchanges over the domain boundaries and a trapezoid-shaped porous region was set on the bottom half of the domain. The solution yielded by the proposed model and the one using drag terms were fairly similar when adjusting the drag coefficients and comparing the velocity and pressure fields over the whole domain, evidencing that large eddies being constricted by the porous media geometry. However, both models differ at the water sediment interface, thus, the interaction between the surface turbulent region and the porous media.

A second experiment taken from an experimental setup was adopted where a constant inflow

of surface water traveled over a set of sand dunes. Both cases yielded different results when analyzing the velocity fields resulting for each one of the realizations, leading to conclude that Drag-NS models cannot always represent the same results that the diffusive model can achieve. In the discussion section, it is argued that the reason for this disagreement between the two models is a result of the incapability of the Drag-NS model to recreate changes in the velocity field due to concavity differences and non-zero boundary conditions rather than changes proportional to the velocity function sign, being inevitably conditioned to the initial conditions given to the problem. Lastly, a comparison between the experimental results of a dye tracer and a scalar transport equation solved for both models was made for qualitative comparison purposes. Our results suggest that both models are useful for assessing the general behavior and flow patterns of the interaction between the surface water and the groundwater in coupled system as rivers and sediment beds.

Further work can be focused on developing the proposed model to take into account effects of anisotropy and to get a clearer relationship between hydraulic conductivity and the apparent viscosity used in this work to characterize the riverbed.

5 Combining Hyporheic Hydrodynamics and Fine Sediment Deposition

After exploring two continuum eulerian modeling approaches, this chapter presents a Lagrangian method to model Hyporheic Flow and its application as a proxy for estimating fine sediment deposition in experimental flumes. Results suggest that for sand beds, the Advective Pumping Model is the most suitable for representing Hyporheic Flow. Moreover, fine sediment deposition is well represented by a first ordering filtration.

1

Fine particle deposition within river beds plays a major role in riverine ecology and biogeochemistry by altering hyporheic exchange flux. Moreover, it is ubiquitous within streams and rivers across all flow stages. However, the dynamics of fine particle deposition are still not completely understood in rivers, and continuum models like the Advection Dispersion Equation require modifications to represent the processes accurately. To enhance understanding of fine particle dynamics, we developed a novel numerical Particle-Tracking model that simulates fine particle deposition as a stochastic process under losing, neutral and gaining streamflow conditions. These flow conditions generate three different velocity profiles by combining the free surface and groundwater flows. In addition, a novel aspect of our model is the storage of filtered particles to estimate concentration fields within the bed. Our simulated results are qualitatively compared with previous laboratory flume experimental results of kaolinite deposition under similar conditions. The model indicates that fine particle deposition patterns and residence time functions depend heavily on the exchange flux between stream and groundwater, as well as bed filtration properties as the deposition of particles occurs at greater depths in the losing stream condition than in the neutral and gaining cases.

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Therefore, the spatial pattern of particle deposition is a direct result of porewater velocity profiles, while the concentration depends on filtration dynamics within the bed.

5.1. Introduction

Rivers integrate over a host of catchment processes representing collections of different geological, biological, chemical and ecological phenomena (Boano et al., 2014). Many of these phenomena depend on the exchange of momentum, matter and energy between the river and the underlying sediments (see Boano et al. (2014) and references therein). Streamflow into and back out of the subsurface is commonly termed hyporheic exchange (HE), and can occur across a range of different scales with varying magnitudes (Stonedahl et al., 2010; Buendia et al., 2014). HE is affected by fine particle transport and deposition within the stream because of filtering processes present in the river bed that can lead to clogging and siltation (Crenshaw et al., 2002; Mendoza-Lera et al., 2017; Fox et al., 2018). This interaction between sediment transport and deposition can alter nutrient fluxes in rivers and plays an important role in determining the integrity of the aquatic ecosystem as a whole (Partington et al., 2017). Indeed, contaminant transport and carbon and nutrient dynamics are closely related to HE and sediment deposition (Hope et al., 1994; Gottselig et al., 2014).

Fine particle deposition, ubiquitous within rivers systems is driven by the interactions of surface flow and bed morphology (Packman et al., 2000b,a; Harvey et al., 2012). Suspended particles in rivers are typically minerals or aggregations of organic matter with sizes smaller than $10\ \mu\text{m}$ (Huettel et al., 1996; Harvey et al., 2012; Drummond et al., 2014, 2018; Jin et al., 2019). Fine particles, due to their small size and density are easily suspended in water (Packman et al., 2000b). However, they may deposit through interactions with geomorphic features which induce hyporheic flow such as dunes, pools, riffles, and bars (Buendia et al., 2014). Moreover, they are well known to deposit in the stream bed and resuspend into the surface flow with some periodicity (Cushing et al., 1993; Newbold et al., 2005; Karwan and Saiers, 2012; Drummond et al., 2015) depending on variations of surface flow conditions, which can be driven by natural floods or the release of water from dams (Drummond et al., 2017). Additionally, fine particle retention in the stream bed is known to affect hyporheic flow, the exchange of nutrients, and alter physical properties of the media like porosity and permeability (Thomas et al., 2001; Crenshaw et al., 2002; Packman and MacKay, 2003; Newbold et al., 2005; Karwan and Saiers, 2009; Dong et al., 2012; Simpson and Meixner, 2012; Mendoza-Lera et al., 2017).

Enhanced fine particle loading in streams and thus increased deposition has recently been fostered by land use changes (Gartner et al., 2012; Wohl, 2015). This increased deposition impacts biogeochemical processes such as nutrient and carbon cycling (Hope et al., 1994; Gottselig et al., 2014) through the reduction of HE as particles clog the river bed (Brunke, 1999). Indeed, fine particle deposition and transport affects the growth of microbial communities and favors denitrification processes due to the lack of oxygen in clogged zones (Navel et al., 2011). Thus, the understanding of fine particle dynamics in riverbeds is a challenge for river restoration and management.

In part due to the complexity of natural rivers, laboratory experiments have represented one of the primary tools for understanding the coupling between HE and sediment deposition (Elliott and Brooks, 1997a; Marion et al., 2002; Salehin et al., 2004). An important insight gained from early experimental efforts suggests that fine particle deposition occurs not only by gravitational deposition (Vanoni, 1974), but also other key physical parameters. Flume models are ideal systems for studying local scale processes and isolating specific mechanisms for understanding the coupling between HE and sediment deposition. Understanding the role of regional groundwater patterns that result in losing and gaining flow conditions on fine sediment deposition has, to date, only been evaluated in relatively small number of experiments (Dong et al., 2012; Simpson and Meixner, 2012; Chen et al., 2013).

At the reach scale, the exchange between surface flows and groundwater has been heavily recorded and modeled (Woessner and Woessner, 2000; Cardenas et al., 2004; Cardenas and Wilson, 2006; Harvey et al., 2012; Hester et al., 2013; Fox et al., 2014; Marzadri et al., 2016). The results of these observations and simulations suggest that the river bed acts as a filter that traps a variety of fine particles through different mechanisms (i.e., filtration and straining). Another relevant result is that particle deposition changes the physical properties of the river beds, like porosity and permeability. However, reach-scale models are not able to accurately quantify the effects of groundwater flow on sediment deposition patterns at small scales. Thus, it is necessary to explore further this aspect to validate how the interaction between free surface flow and groundwater flow hinders or fosters sediment deposition in streams.

Particle deposition has been assessed under the assumptions of the advective pumping model in numerical simulations, generating flow paths in the stream bed due to the change of pressure generated by the presence of ripples and dunes (Elliott and Brooks, 1997b,a). Some of these models have focused on estimating hydrodynamic fields and solute transport using continuum mechanics expressions such as the Advection Dispersion Equation (ADE) (Cardenas and Wilson, 2006, 2007a,b; Boano et al., 2007; Cardenas et al., 2008; Trauth et al., 2013). Models that use numerical particles that represent fine sediments have also been used to assess deposition patterns through the use of measured velocity profiles at local scales (Packman et al., 2000b). The particle tracking (PT) approach can also be used at reach scales to model nutrient uptake in rivers (Li et al., 2017). Advantages of using PT models is that this technique is useful for a wide range of scales (Delay et al., 2005), and that physical and chemical processes can be included and analyzed separately. However, modeling the physical process of particle deposition under different groundwater flow conditions remains a major challenge for river systems, since current models do not include explicit terms that account for vertical groundwater flow. Therefore, estimating the effect of particle deposition and HE remains imprecise.

This paper aims to present a particle tracking model that assess fine sediment deposition under losing or gaining stream flow conditions. This is a novel approach, since it explores the macroscopic process of flow in porous media due to the advective pumping model and through the incorporation of a discrete probabilistic framework that simulates the filtration process within the bed. By implementing this model, new information is gained regarding

on the accumulation patterns of particles under neutral, upflow, and downflow conditions. Moreover, these results show that our model can be used as a direct comparison of fine particle deposition in systems with regular sand beds under losing and gaining streamflow conditions.

5.2. Methods

5.2.1. Conceptual model

The particle tracking model aims to represent instantaneous fine sediment deposition dynamics within an idealized sand-bed with periodic bedforms and variable groundwater flow patterns (figure 5-1). The conceptual model framework follows the work by Elliott and Brooks (1997b,a); Packman et al. (2000b); Packman and Bencala (2000), while the groundwater flows represent conditions that were used in the experimental setup within the work of Fox et al. (2014, 2018). Our numerical PT model builds on the framework of Li et al. (2017) developed to understand nutrient transport in rivers. However, for this case the particles are recorded at every timestep to assess the deposition patterns within the domain. Here we impose a gaining or losing flux at the bottom of the model domain as a superposition of the velocity field generated from the advective pumping model (Elliott and Brooks, 1997b). The geomorphological and hydrologic flow conditions within the numerical model most closely represent a two dimensional simplification of the experimental conditions within previous studies on fine particle deposition (Packman et al., 2000b; Fox et al., 2014, 2018)(table 5-1). However, these features are fairly typical of natural sand bed systems (Vanoni, 1974; Harvey et al., 2012; Wörman et al., 2007; Hünken and Mutz, 2007; Mutz, 2000; Mutz and Rohde, 2003; Dong et al., 2012; Simpson and Meixner, 2012; Chen et al., 2013). To further generalize the model, non dimensional quantities are used for the comparisons.

The primary assumptions within the model are (i) macroscopic processes are considered separately from pore-scale processes, hence the movement of the particles is considered independent from the bed filtration process; (ii) particles do not interact with each other; (iii) particles do not change the flow conditions in the media when they are filtered in the bed; (iv) fine particle deposition is irreversible; and (v) the shape of the dune is replaced by a sinusoidal pressure applied at the top of the domain. From experiments we know that these assumptions are not always valid, as particle collisions can lead to larger agglomerates and particle clogging can alter flow paths (Fox et al., 2018). However, since the particle injection is instantaneous and the flow conditions are permanent, alteration of the velocity field is not taken into account. In the case of a continuous particle injection, the alteration of flow paths would depend on particle deposition through a feedback cycle between the velocity field and filtration within the domain.

The horizontal model computational domain represents a single dune wavelength (λ) (figure 5-1). In the vertical axis, the domain has a side d_b that stands for the depth of the sand bed, or the distance between the free surface flow and an impervious layer at the bottom of the domain. For practical purposes the width of the sand bed was modeled according to

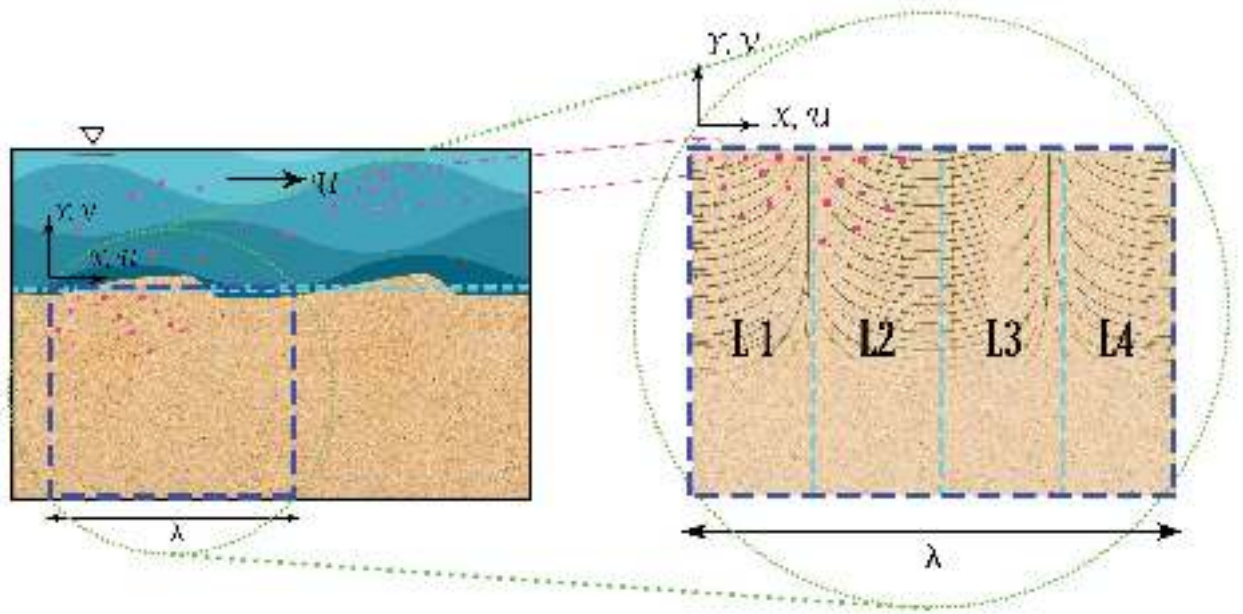


Figure 5-1: Conceptual model. Left: Sand bed with dune-shaped bedforms. The blue box outlines the model domain (λ is the characteristic dune's wavelength). The cyan dashed line demarcates the mean height of the bed. Right: Zoom of the model domain. Idealized streamlines from velocity profiles. Note that the lateral boundary conditions of the model are periodic. Particles (pink rectangles), are seeded at the top of the domain in the left half of the dune, propagate through the bed, and are filtered within bed sediments. The domain is divided into four locations (L1 to L4) to compare the deposition patterns with the experiments from Fox et al. (2018).

Table 5-1: Physical parameters (Packman et al., 2000b; Fox et al., 2014, 2018) for the comparison of the implemented Particle-Tracking model.

PHYSICAL PARAMETERS	SYMBOL	VALUE
Flume width [<i>cm</i>]	W	29.0
Sediment porosity $[-]$	θ	0.33
Hydraulic conductivity [<i>cm/s</i>]	K	0.12
Flow [<i>l/min</i>]	Q	261.0
Mean stream velocity [<i>cm/s</i>]	U	15.0
Sediment depth [<i>cm</i>]	d_b	20.0
Dune wavelegth [<i>cm</i>]	λ	15.0
Water depth [<i>cm</i>]	d	8.8
Total streambed area [<i>cm</i> ²]	A	15.1
Imposed vertical flux (in/out) [<i>cm/d</i>]	q_{in}	$\pm 12,5$
Filtering coefficient [<i>1/cm</i>]	λ_f	0.6

experimental values reported (Fox et al., 2014, 2018). The sides of the box are open and they represent periodic boundary conditions as particles that exit the domain on the right will re-enter on the left boundary and vice versa (figure 5-1).

The free surface model flow conditions are approximated by combining the advective pumping model (Elliott and Brooks, 1997b) with each groundwater flow condition (i.e., losing, neutral or gaining). This model estimates the velocity field within the bed as a result of pressure variations at the top of the sand dunes that form the river bed. The particles are seeded at the top of the domain in the left half ($\lambda/2$), which conceptually represents the upstream (stoss) side of the sand dune. The particle injection is instantaneous and performed before the first timestep of the model. Each timestep, the introduced particles travel according to the estimated velocity field followed by a filtration step represented as a random process. Subsections 5.2.2 and 5.2.3 explain in detail the particle mobility and trapping/filtering features of the model.

5.2.2. Mathematical Model

The velocity fields used to model the water flow inside the dune are taken from existing literature (Elliott and Brooks, 1997b; Packman et al., 2000b) with an additional superimposed groundwater flow component (equations 5-1 and 5-2). The groundwater vertical flow condition represents a positive upwards velocity for the gaining condition and negative downwards velocity for the losing condition.

$$u(x, y) = -(kKh_m) \cos(kx) [\tanh(kd_b) \sinh(ky) + \cosh(ky)] , \quad (5-1)$$

$$v(x, y) = -(kKh_m) \sin(kx) [\tanh(kd_b) \cosh(ky) + \sinh(ky)] \pm q_{in/out} , \quad (5-2)$$

Where x and y represent the Cartesian coordinate reference axis ($x > 0$ for the downstream direction and $y = 0$ at the top of the domain), k is the normalized dune wavelength ($2\pi/\lambda$) and u and v are the horizontal and vertical velocity components, respectively. Furthermore, h_m represents the mean pressure over the dune, K stands for the permeability of the media, d_b for the thickness of the bed and $q_{in/out}$ is the component of vertical velocity caused by the groundwater inflow/outflow.

We normalized all of the quantities and parameters according to theory developed for flow and transport in sand beds (Elliott and Brooks, 1997b; Packman et al., 2000b). As a result, equations 5-1 and 5-2 are transformed in equations 5-3 and 5-4. The inflow/outflow velocity $q_{in/out}$ is normalized by the maximum pumping velocity u_m . The addition of the vertical velocity alters the flow directions within the domain and introduces areas of flow recirculation and stagnation absent in the neutral flow condition velocity profiles (figure 5-2a-c). The neutral velocity profile (figure 5-2b) shows streamlines starting and ending in two vertical streamlines that enter and leave the domain at $-\pi/2$ and $\pi/2$. For the losing flow condition (figure 5-2a) the vertical streamline that enters the domain at $\pi/2$ remains unaffected in its shape. However, the vertical streamline at $-\pi/2$ is shortened due to the presence of the downward imposed flux. This feature generates a recirculation zone that enhances vertical downwards flux and hinders the upward flux that leaves the domain. Instead, for the gaining flow condition (figure 5-2c), the vertical streamline located at $\pi/2$ going downwards is shortened and the streamline at $-\pi/2$ going upwards is enhanced by the groundwater flow condition.

$$u^*(x^*, y^*) = -\cos(x^*) [\tanh(d_b^*) \sinh(y^*) + \cosh(y^*)] , \quad (5-3)$$

$$v^*(x^*, y^*) = -\sin(x^*) [\tanh(d_b^*) \cosh(y^*) + \sinh(y^*)] \pm q_{in/out}^* , \quad (5-4)$$

The resulting velocity fields generated with the superposition of the advective pumping model and the vertical groundwater flow are physically reasonable, as the lowest velocities are present at the bottom of the domain where the influence of the surface flow has been reduced and the vertical groundwater flow prevails. At the top of the domain, the opposite happens, i.e. the flow field is highly affected by surface flow conditions and the effects of the imposed groundwater flow are less evident. We can assess the particle path behavior relative to the velocity profiles through the Stokes number, which is defined as the relation between the stopping distance and the characteristic length of the phenomenon (equation 5-5) (Ren and Packman, 2002; Clark, 2009).

$$Stk = \frac{\rho_p d_p^2 u_0}{18 \mu_f l_0} , \quad (5-5)$$

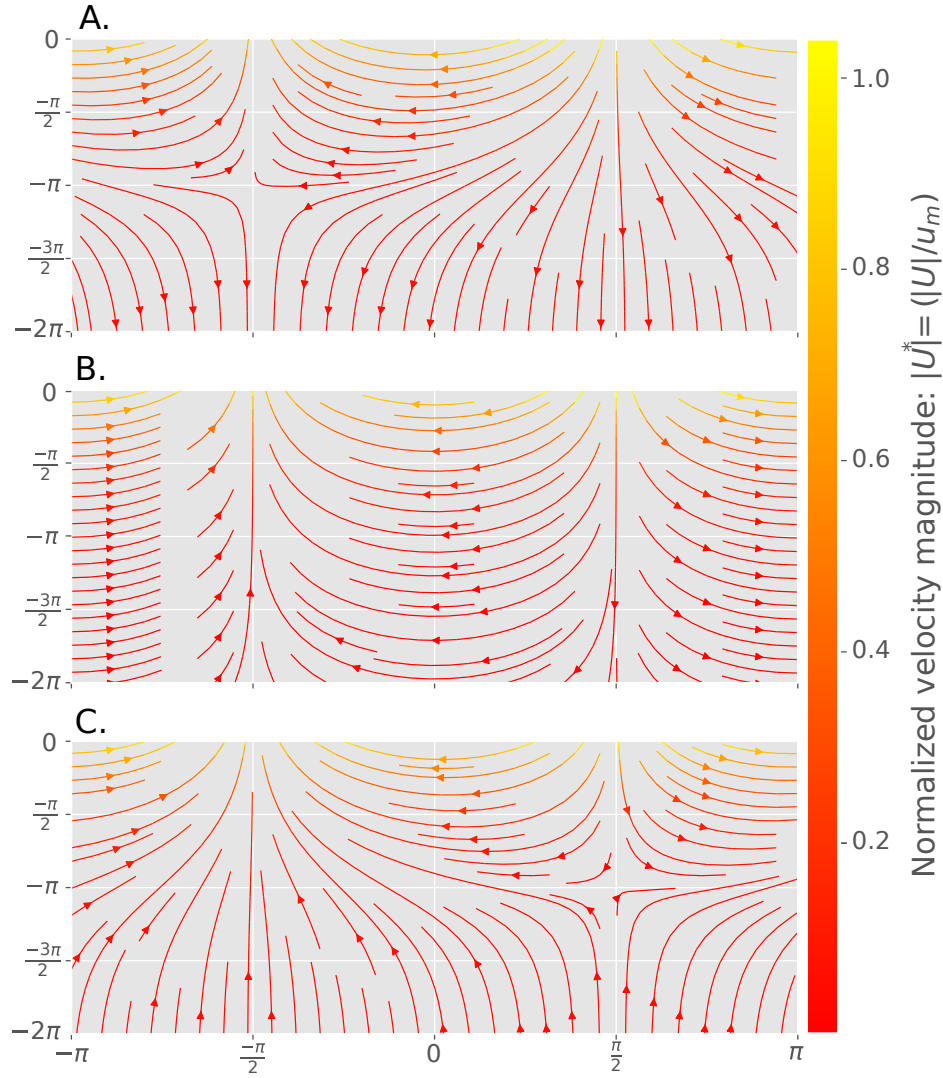


Figure 5-2: Streamlines for Losing (A), Neutral (B) and Gaining (C) flow conditions. Domains are plotted in the interval $[-\pi/2, \pi/2]$ as each domain is periodic. The color bar represents the magnitude of the velocity vector. Vertical and horizontal axis not to scale.

where ρ_p is the particle density taken here as that of kaolinite (2650 kg/m^3), $d_p = 384 \times 10^{-6} \text{ m}$ is the mean diameter (Fox et al., 2014), $u_0 = 0,01 \text{ m/s}$ is the mean velocity in the subsurface, $\mu_f = 1,519 \times 10^{-3} \text{ Pa s}$ is the dynamic viscosity of water (Cengel and Cimbala, 2006), and $l_0 = 0,01 \text{ m}$ is a characteristic length of the phenomenon which is taken as the dune's height (Fox et al., 2018). With a Stokes number $Stk = 0,014$ less than 1.0 we expect clay particles to follow streamlines and thus our model particles track the velocity profile streamlines described in equations 5-3 and 5-4 (Tropea et al., 2007). Settling velocity is neglected for this experiment under the assumption that particle diameters are small and enter the bed at low velocities to ensure a low Stokes number such that they will follow the streamlines generated by the velocity fields (Ren and Packman, 2002). While not implemented here, the model framework is able to take into account this feature. The mathematical model starts with the transport of particles along given streamlines, i.e. the Advection Dispersion Equation (ADE) (equation 5-6).

$$\frac{\partial C}{\partial t} + u(x, y) \frac{\partial C}{\partial x} + v(x, y) \frac{\partial C}{\partial y} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) - S, \quad (5-6)$$

Here, C stands for the concentration of the particles, u and v for the horizontal and vertical velocities, respectively; D for the mechanical dispersion coefficient and S for rate of particles removal due to filtration (Packman, 1997). The dispersion process for colloids with diameters $< 2\mu\text{m}$ can be neglected in particle transport in porous media (Domenico and Schwartz, 1998; Packman et al., 2000b; Ren and Packman, 2002; Boano et al., 2014). Therefore, the ADE can be transformed into an equation that represents a filtration process over a given velocity field (equation 5-7). Here, the local and advective acceleration equal the rate of removal of particles over time.

$$\frac{DC}{Dt} = \frac{\partial C}{\partial t} + u(x, y) \frac{\partial C}{\partial x} + v(x, y) \frac{\partial C}{\partial y} = -S, \quad (5-7)$$

The rate of particle removal S can be expressed with the aid of the filtration coefficient λ_f , the seepage velocity $U = \partial s / \partial t$ (where s is the path traveled by the particle), and the concentration C of the analyzed particles as follows:

$$S = \lambda_f \frac{\partial s}{\partial t} C, \quad (5-8)$$

Combining 5-8 with equation 5-7, the expression for particle filtering becomes:

$$\frac{\partial C}{\partial s} = -\lambda_f C, \quad (5-9)$$

This model formulation is consistent with previous models of colloidal transport in porous media (Domenico and Schwartz, 1998). The key outcome of the mathematical model is that a filtration process along steady streamlines can be expressed as a first order removal rate. In other words, the stochastic framework for filtration is applied using a removal constant (λ_f) to estimate the probability (p) that each particle has been filtered while traveling along a flow path (see section 5.2.3).

5.2.3. Numerical Model

The proposed numerical model is similar to the one used by Packman et al. (2000b). Its logical process is divided in three parts that use the discrete versions of equations 5-7 and 5-9. The initial step calculates the displacement of particles using the Taylor series expansion $x(t + \Delta t) = x(t) + u \cdot \Delta t$ (Li et al., 2017). Each timestep the model takes into account the particles' previous positions and determines their velocities based on the velocity field.

After estimating each particle's position, the filtration process over the timestep is estimated by calculating the probability p that the particle stops inside the domain (Prickett et al., 1981). This is provided by generating a random number (n) for each particle and comparing the random number with the λ_f and the distance traveled by the particle over the timestep (Δs).

$$p = 1 - e^{-\lambda_f \Delta s} \approx \lambda_f \Delta s, \quad (5-10)$$

This assumption is justified as the size of the timestep Δt is small enough to ensure the validity of the Taylor's expansion (Li et al., 2017). At the end of every timestep particles within the domain are counted and divided into two categories: (i) filtered particles that will remain immobile for the remainder of the simulation; and (ii) mobile particles which have not been filtered. Particles that leave the domain out of the top boundary are accounted for as escaped particles that do not return to the domain during the simulation.

The particle-tracking simulations were performed under the conditions proposed in table 5-1. The cases were modeled with 2×10^5 particles for each vertical flow condition (Losing, Neutral and Gaining). The total simulation time ensured that all of the seeded particles were either filtered or escaped the domain by the end of the simulation. As regards to the initial condition, the particles are seeded uniformly across the left half of the top of the domain ($0 < x^* < \pi$) within the imposed downwelling flow due to HE. Particles are not seeded on the right part of the domain ($\pi < x^* < 2\pi$) as the upwelling flow from HE would result in these particles immediately escaping the domain 5-2.

To compare the PT model with the experimental results (Fox et al., 2014, 2018), the model domain is superimposed with a mesh of 100×167 squares of size $\pi/50$. Then, particles are binned and counted in each square. The resolution of the mesh was selected according to the experimental framework to be able to compare the number of particles in our model with clay concentration of the experiments. It is worth mentioning that the mesh used for

counting particles has no relationship with the computational PT simulation as it is only used for particle counting purposes (Xue et al., 2017).

The numerical model is implemented in Matlab via a primary script that performs the individual particle tracking and stores the particles' locations in a range of time selected by the user. For the case of each model run, particles' coordinates were stored every ten timesteps. After the particle tracking model run, the output coordinates are read by a Python script that counts particles inside the superimposed mesh to generate particle maps and process information over space and time. The primary results that are analyzed are from particle counting rather than the raw PT model results. Model codes are freely available (see acknowledgements).

To estimate the Residence Time Function (RTF), i.e., the fraction of particles injected in the bed at a time t_0 and still present within the domain in a given time t (Packman et al., 2000b), particles are separated into three categories during a run: i) traveling particles, ii) filtered particles and iii) particles that escaped the domain. For any given timestep, the RTF is the result of sum of particles that are traveling through the domain with the particles that have been previously filtered. The result is then normalized by the total number of particles seeded at the beginning of the model.

5.3. Results

The porewater flow patterns under losing, neutral and gaining streamflow conditions that result from equations 5-3 and 5-4 show substantial differences (figure 5-2). Preferential flow paths going upwards or downwards occur when the imposed condition is a gaining or losing flow, respectively. The addition of vertical flow (losing/gaining) to the neutral flow condition creates an area of no net flow across the sediment-water interface (SWI) that corresponds to the top part of the domain. For the losing case, this area is located at the lee side of the dune ($-\pi/2$), and for the gaining condition on the stoss side ($\pi/2$). In these areas there is no flow at all because of the superposition of the advective pumping model with the groundwater vertical flow condition. In addition, the areas of no flow create a corresponding recirculation zone in the losing and gaining cases (locations can be seen in Figure 5-2A in the coordinates $(-\pi/2, -\pi)$ and C in the coordinate $(\pi/2, \pi)$). These recirculation zones are expected to trap any particles that are able to reach them.

Due to the altered losing and gaining flow conditions, the maximum velocities in each profile are located in different places. In particular, in the losing condition the maximum velocity is into the bed (negative) on the stoss side (upstream) of the domain, while in the gaining case it is located in dune's lee (downstream). However, in the neutral condition the maximum velocities are located in two parts of the domain but with opposite signs, with downwelling on the lee ($-\pi/2$) and the upwelling on the stoss ($\pi/2$) side. Even though particles follow the streamlines of the porewater flow patterns, their deposition is not uniform due to the inflow position on the upstream side of the dune's stoss side and filtering along the streamlines.

During early simulation times, the fine particle deposition patterns are generally similar in

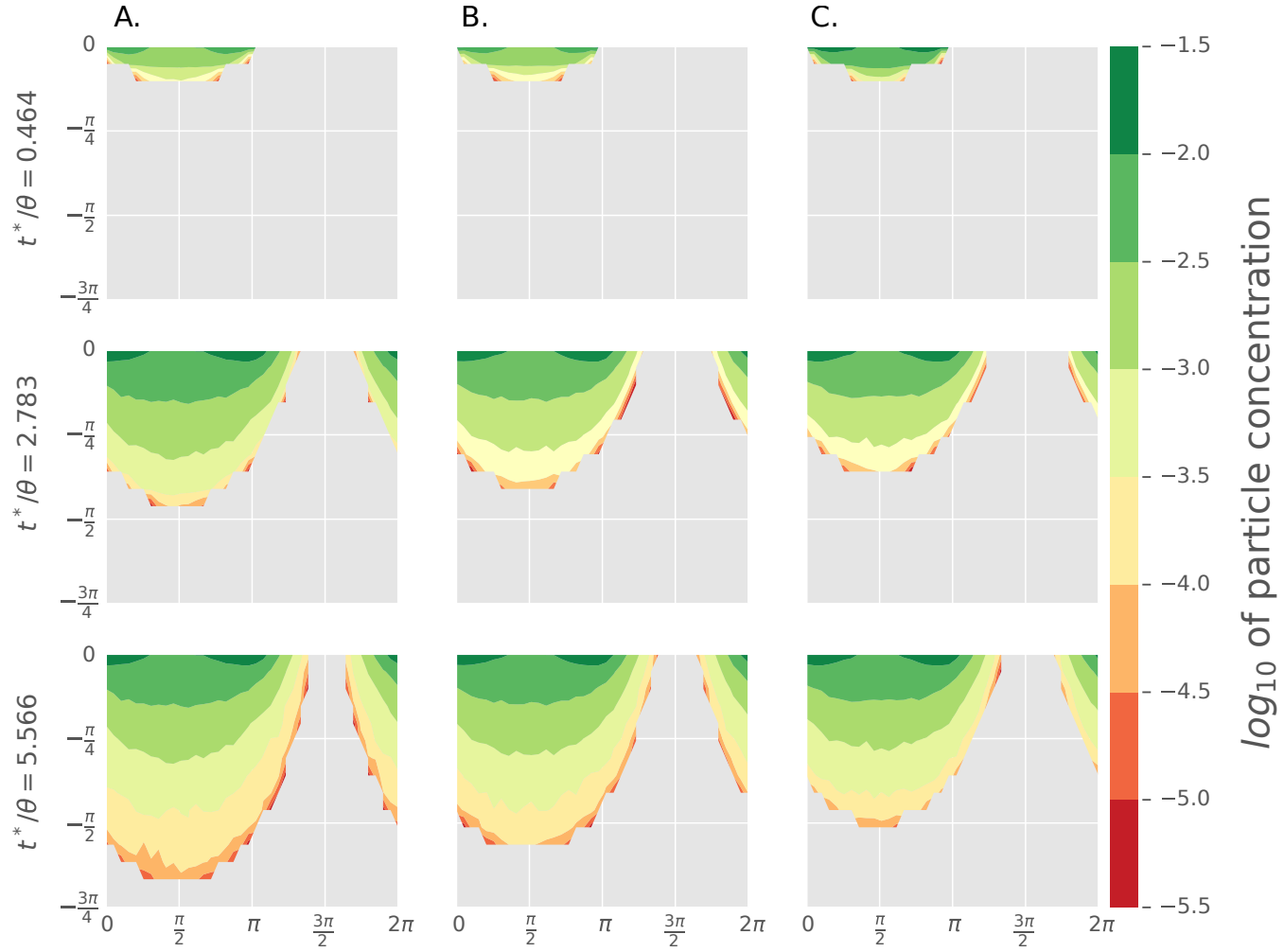


Figure 5-3: Logarithm of the total number of particles deposited for different times (rows), and under different inflow/outflow conditions (columns). (A) Losing condition, (B) Neutral condition and (C) Gaining condition (Note that axis are not to scale).

shape for the three modeled cases, though the concentrations differ (figure 5-3 first row). For example, in the gaining condition the particles in the uppermost part of the domain are more evenly distributed than in the neutral and losing cases. At later times, the flow pattern due to advective pumping remains prominent as the area of return flow is free of particles. However, the distribution of return flow is modified by the imposed vertical flow conditions; in the losing case it is significantly narrower than in the neutral and gaining ones (figure 5-3).

With the PT model we can assess the particles behavior over time (figure 5-4), because we record the relative number of mobile, filtered, and escaped particles within the domain (figure 5-4). Even though each flow condition has the same filtration coefficient, the amount of particles that remain in the domain and escape from it varies appreciably between the imposed vertical flow conditions. Each one of the vertical flow conditions has characteristic curves of filtered, mobile, and escaped particles (figure 5-4). For the losing case the fraction of filtered particles at the end of the simulation is 0,82; while it is 0,78 and 0,76 for the neutral and gaining cases, respectively. Conversely, 0,17, 0,20 and 0,24 of particles escaped the domain under the losing, neutral and gaining cases, respectively. The behavior of the escaped, mobile, and filtered particles over time presents the same pattern between flow conditions, although there is a marked delayed onset of escaping particles in the losing flow condition. For gaining flow, however, some particles are initially lost upon seeding because they are carried out of the bed by upwelling water. In particular, the filtered particles present an exponential behavior in time, while the traveling and escaped particles have a monotonic increase until reaching a peak.

The PT model recovers the expected ensemble continuum behavior of fine particle deposition. The filtration process is expected to remove particles in an exponential way as a function of distance traveled by each particle, and this phenomenon is present in the model results. However, the presence of particles inside the domain is heavily conditioned by the vertical groundwater flow imposed. By tracking the number of remaining particles within the PT model we can estimate a Residence Time Function (RTF). The three RTF were calculated as the fraction of particles that enter the bed near $t = 0$ and remain inside the domain after a given time τ (Elliott and Brooks, 1997b; Packman et al., 2000b). For small times, τ close to zero, the value of the RTF is 1,0; as τ increases some of the particles leave the domain and the RTF begins to decrease. Since the RTF is normalized by the total number of particles (figure 5-5), the resulting curve is the complement of the cumulative distribution function ($1 - CDF$) of particles inside the domain.

The number of particles remaining within the domain depends on the vertical flow conditions. Neutral and gaining flow conditions have RTFs with very similar shapes, although under gaining flow fewer particles enter the bed from the start. Unlike the neutral and gaining flow conditions, under losing flow the RTF remains constant for a short period where all particles enter the bed and none have escaped yet. At longer timescales each RTF approaches a constant value. Although gaining and losing conditions have the same imposed flow speed but a different direction, the results of the RTF for the losing and gaining conditions are vertically shifted versions of the RTF curve of the neutral condition. To explore this, the

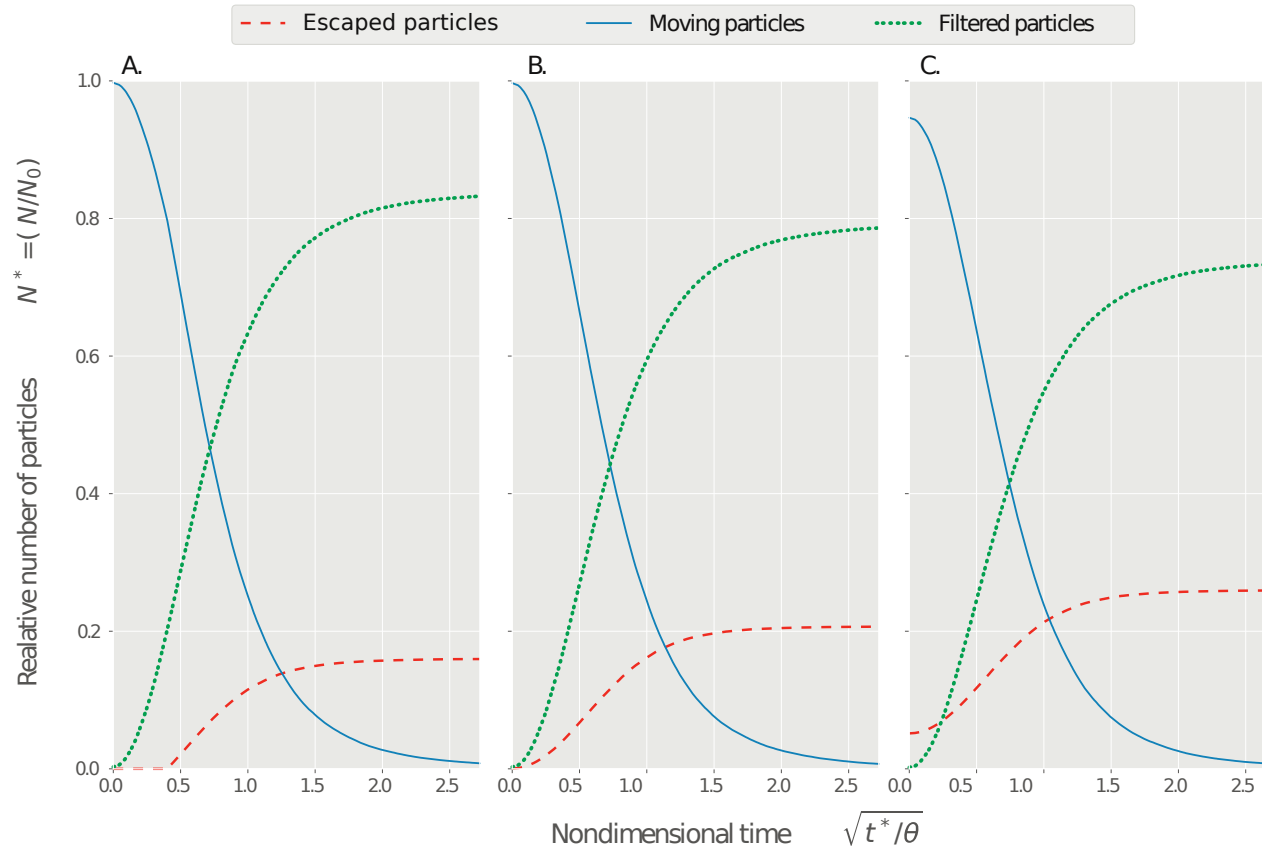


Figure 5-4: Behavior of escaped (dashed Red line), moving (solid blue line), and filtered (dotted green line) particles over time. (A) Losing condition. (B) Neutral condition and (C) Gaining condition.

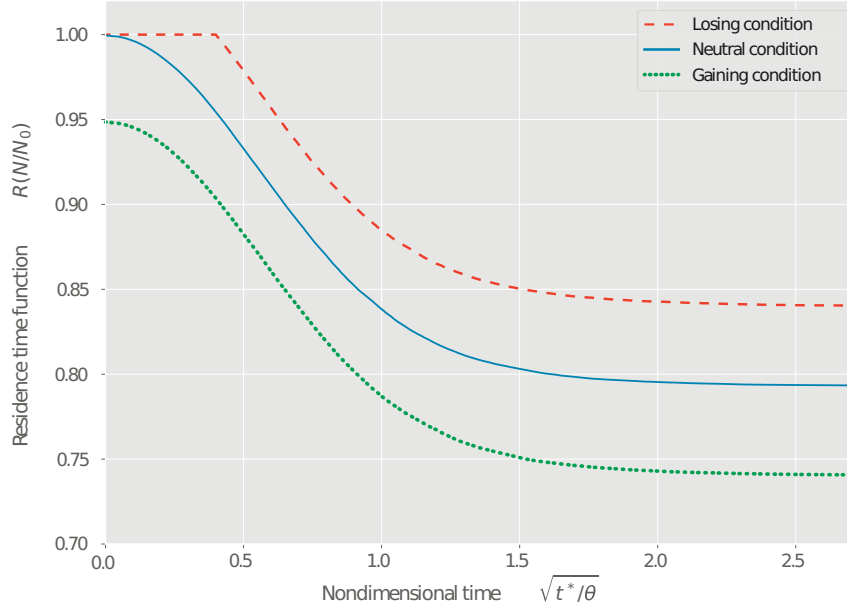


Figure 5-5: Residence time function for the different imposed flow conditions. The lines represent the complement of the Cumulative Distribution Function ($1 - CDF$) of particles inside the domain at a time t^*/θ after the injection.

Residence Time Distributions (RTD) for each time (figure 5-6) were obtained by taking the gradient of each RTF and then applying a convolution between the derivative and a top hat function with unit area and a span of 400 points.

For all modeled cases, the probability of a particle leaving the domain is low at early times followed by an increase until the peak and then a monotonic decrease until all particles are removed or filtered. The time it takes the RTF to decrease at early times corresponds to the minimal path that a particle travels through the domain before exiting at the surface. For the losing case, this path is longer than for the neutral and gaining cases. Therefore, particles tend to remain inside the domain for more time, traveling longer distances inside and are more prone to remain inside the domain (figure 5-6 red line). This means that the probability of leaving the domain is lower for this case than for the neutral or gaining cases until reaching its peak value, again lower than for the two aforementioned cases. The primary difference between the three conditions occurs before the peak in the RTD probability, after this point the three distributions are nearly identical (figure 5-6).

We compare the PT model output with the experimental results from Fox et al. (2014, 2018). Experimental subsurface particle accumulation was sampled by coring each dune in triplicate at four equally spaced locations (5-1c). Kaolinite mass was measured from the extracted cores at 0,5 cm intervals for each location. To facilitate the comparison between the experimental results and the PT model, we divide the non-dimensional domain into sections of $\pi/2$ width. We then calculate the mean and standard deviation of the fraction of

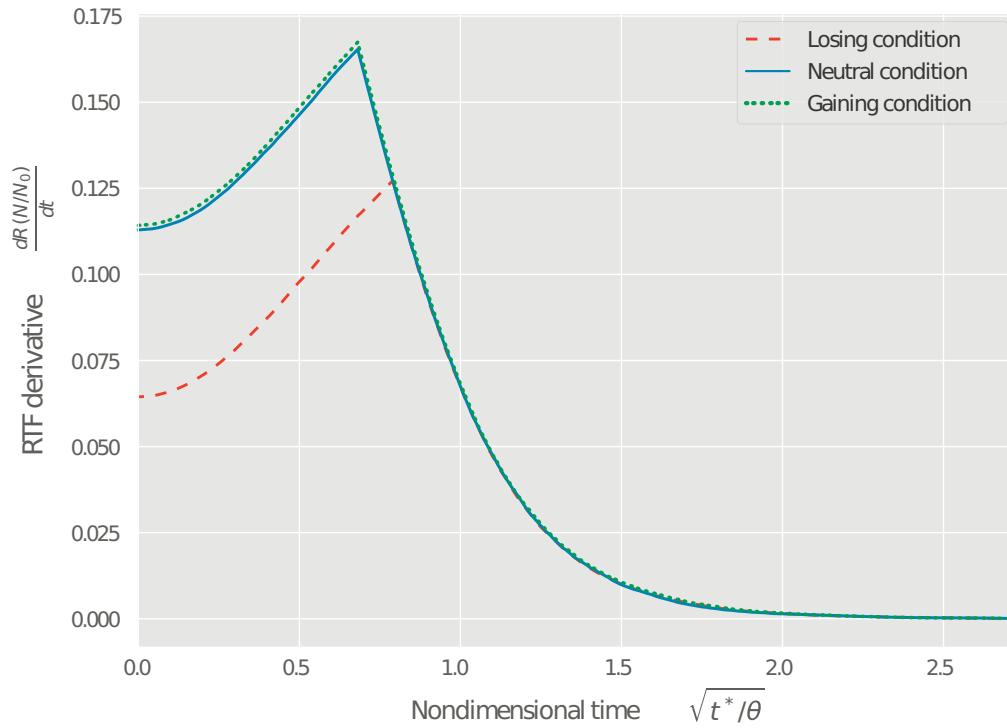


Figure 5-6: Derivative of RTF for the three vertical groundwater flow conditions modeled. These lines represent the Probability Density Function (PDF) of particles inside the domain at a given time t^*/θ after injection

particles at each location (L1, L2, L3 and L4 from figure 5-1) and compare the mass fraction of clay with the fraction of particles in every location (figure 5-7). Our results show strong similarities with the experimental results. Particles deposit more in locations one and two (the stoss side of the dune), and show reduced deposition in locations three and four (lee side of the dune). The deposition in the latter locations occurs due to the particles following the hyporheic flow paths (figure 5-2). There is good agreement between the PT model and the experimental results in the stoss of the sand dune (figure 5-7 first two columns, locations 1 and 2 in right part of figure 5-1). For each of the three flow cases modeled, the PT model underestimates the concentration of particles as the experimental results show more clay deposited with depth for locations three and four (figure 5-7).

5.4. Discussion

The PT model developed here combines a continuum Advective Pumping hyporheic flow model with a stochastic filtration framework to simulate fine particle deposition within a sand bed. This is a novel approach that allows quantification of the fraction of mass deposited within a typical dune under homogeneous flow conditions. The superposition principle could be applied to estimate deposition behavior under different flow and injection conditions. Therefore, our results suggest that the model may be able to capture the macro-processes of fine sediment deposition under losing, gaining and neutral conditions. Additionally, our PT model framework does not pose any problems regarding mass conservation, artificial diffusion or unwanted oscillations provoked by numerical scheme instabilities (Delay et al., 2005). The particle deposition and flow patterns are consistent with experiments and follow the expected mean continuum behavior, i.e. our model captures the physical processes in a representative scale by simulating the combination between the pore scale filtration and the macro scale advective pumping flow. Additions to the current modeling framework can be used to explore in further detail fine particle deposition phenomenon and patterns.

The Stokes number for each individual particle is low enough that it is safe to assume that the particles follow the streamlines. This assumption is supported due to the size of a typical clay particle and the maximum velocity which it is subject to when entering the streambed. Since the low Stokes number assumption is validated for the maximum velocity, it holds for all lower velocities (equation 5-5). Consequently, the phenomenon of settling velocity inside the sand bed is not taken into account as it was in previous works (Packman et al., 2000b; Jin et al., 2019).

The gaining flow condition produces less deposition than the neutral and losing condition (figure 5-3). At early times the deposition is similar for all of the three modeled cases because the shallow streamlines have higher velocity, hence they are barely altered by the groundwater flow. However, when particles travel to deeper parts, the groundwater and vertical flows become more important. The groundwater vertical flow imposed is estimated to be 8 % of the maximum pumping velocity u_m at the top of the domain. However, filtration is a function of each particle's displacement s , hence deposition occurs primarily at the top of the domain in all of the modeled cases, because of the combination of velocity profiles

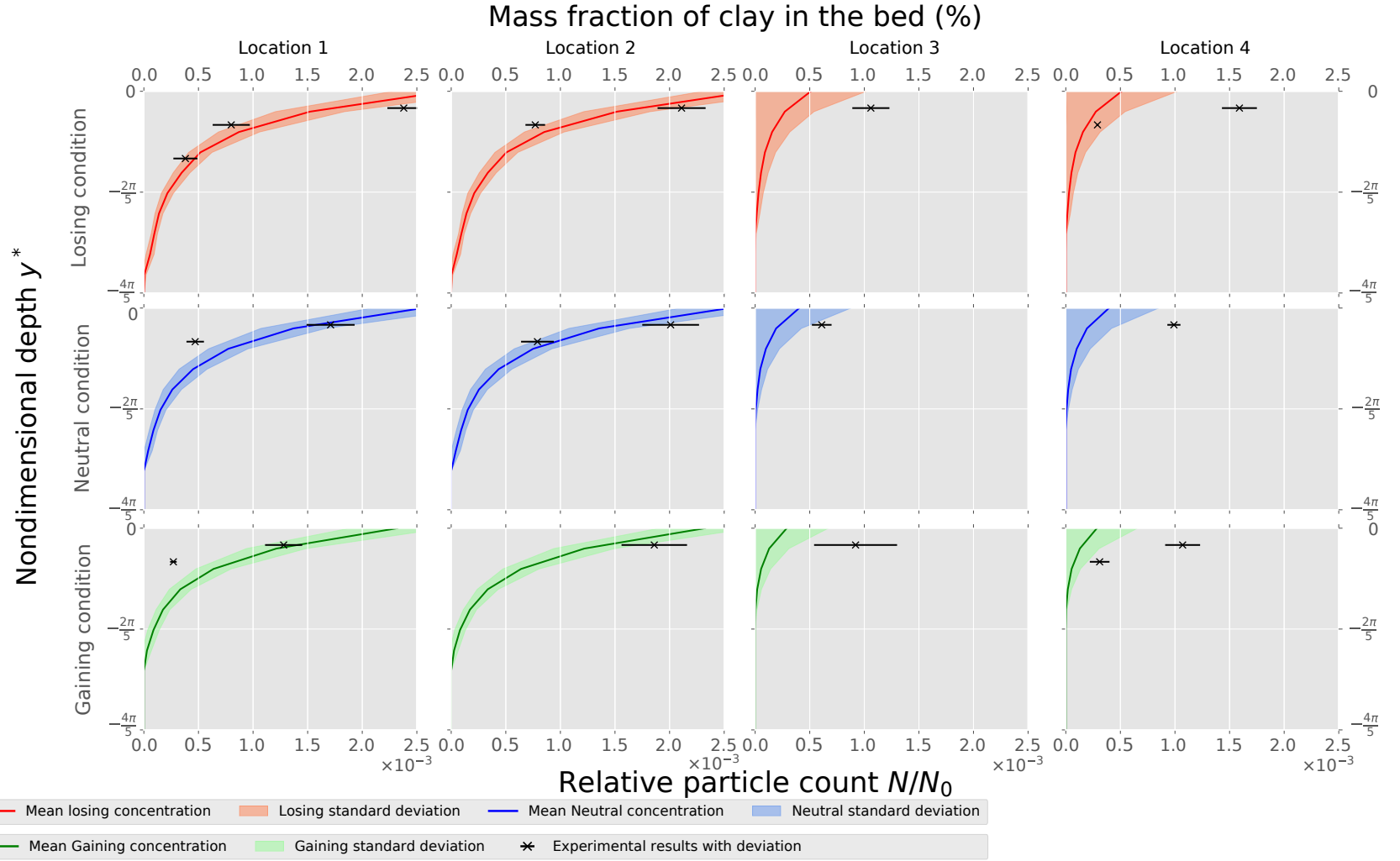


Figure 5-7: Comparison with experimental results from (Fox et al., 2018). The top horizontal axis represents the fraction of clay mass found in the experiments expressed in %. The bottom horizontal axis represents the fraction of particles within the numerical domain. Solid colored lines and their corresponding shaded areas represent the average fraction and standard deviation of particles at each depth for the different locations. Crosses are the mean mass fraction sampled in the experiments, and black lines represent the standard deviation of the measurements.

generated by the dune shapes and the imposed vertical groundwater flow.

Important differences arise when comparing deposition patterns from the three conditions modeled as the depositional pattern depends on the overall combined subsurface velocity profiles. The deposition patterns (figure 5-3), show that a change in the vertical flow conditions affect the maximum penetration depth of the particles, and the horizontal extent of the particles. Not only more of particles deposit under the losing flow condition, but the deposited particles will also cover a larger subsurface volume than the neutral and gaining cases (figure 5-3).

The model-predicted decay of mean clay concentration with depth is similar to the experimental results presented by Fox et al. (2018), especially for the stoss side of the dune. Agreement between the PT model and the experimental results is poorer for the lee side of the bedform and, in general, the PT model standard deviation is less than that of the experimental results. The increased variability within the experimental results may be explained by differences in shape of the dunes in the experiment and the proposed idealized dune within the numerical model. Our model simulates an idealized dune with a fixed shape and constant physical properties inside the domain, while the shape of the dunes and the bed porosity are not homogeneous in the experiments.

The PT model is built on steady, continuum Darcy flow assumptions, hence the effects of turbulent flows on the subsurface velocity patterns are not taken into account. In natural and laboratory cases, some of the total fine particle deposition occurs due to turbulence because of its ability to transport mass and momentum from the free flow stream to the porous media (Roche et al., 2018). Nevertheless, in sand beds the constrained pore spaces damp turbulence, making mean velocity fields and filtration dynamics the main drivers for deposition. This is also a relevant result in the experiments by Fox et al. (2018). However, our model is able to capture the main fine particle deposition phenomenon for this particular type of bed. For the case of cobble-bed flows with bigger spaces between grains, this model would not be suitable since the effects of turbulence from the free flow penetrate the bed, hence presenting unsteady flow effects (Packman et al., 2004; Manes et al., 2011).

In addition, changes in porosity (hence permeability) of the media due to the particles' deposition has been recorded in lab observations and numerical simulations (Chen et al., 2008), affecting the shape of the velocity fields under the different flow conditions. The change of bed porosity hinders HE in rivers and has visible effects on experimental HE patterns (Tonina et al., 2016; Fox et al., 2018). Our model provides a potential basis for simulating clogging processes in sand beds since it tracks the particles' position within the bed following a generated velocity field. However, effects on media heterogeneity are not taken into account within the current implementation. Nevertheless, heterogeneity in the porous medium can be considered using this particle-tracking model approach, but that would require assumptions or observations regarding the structure of the bed and how the filtration coefficient varies within different types of sedimentary deposits. Our model focuses primarily on the main particle transport processes. Therefore complexity associated with river bed heterogeneity is beyond the scope of the current paper. Changes in permeability can be associated with the number of filtered particles within the domain. Afterwards, a

new transient flow field can be estimated to filter the remaining particles that move within the bed. However, there is a second-order effect of particle accumulation in the bed and it is the change in filtration coefficient due to the bed clogging. However, our results suggest that the proposed PT model is suitable to represent deposition patterns under different flow conditions.

Finally, natural streams are characterized by their heterogeneity in space and time, hence our homogeneous sand bed PT model is not able to capture the fine particle deposition when compared to a more complex media made of different stratified materials like the ones found in natural streams. However, our results suggest that PT models remain a good approximation of observed fine particle deposition phenomenon and that this type of model is a good approximation for understanding how combined physical phenomena act as a whole in natural systems. Additionally, the validated behavior of particle filtration and transport within the bed allows for more complex phenomena to be added to the model, such as simulating the effects of chemical gradients or the presence of bio-active layers on non conservative or reactive particles.

5.5. Conclusions

The implemented PT model showed substantial differences in the deposition profiles of fine particles in a sediment bed (figure 5-3). For the gaining flow condition the maximum penetration depth of the particles is less than in the neutral and losing cases, where the velocity fields push the particles further down within the domain. Our results suggest that the model captures the main physical processes of fine particle deposition within a streambed when combining the advective pumping model of a dune shaped bed and the vertical groundwater flow conditions. Besides the maximum penetration of the particles within the domain, their spatial distribution is also different among cases, showing the combination of vertical flow conditions and filtration inside a sand bed. However the particles' dynamics regarding the RTF of each case modeled show similarities, suggesting that the flow field shape and magnitude impact also the velocity of the particles while traveling across the domain. This effect is also seen in the presence of shallow zones with no particles inside the lee side of the modeled dunes. These zones are important for riverine biogeochemistry since they are the not occupied by fine particles that can obstruct the hyporheic exchange in natural systems composed by sand beds. Furthermore, these zones are present in experimental works done previously (Fox et al., 2014, 2018), showing that the proposed model is able to represent complex dynamics of particle deposition with results that are similar to the ones found both in flumes and natural systems.

6 Discussion, Conclusions and Outlook

This chapter aims to connect the results obtained in the previous sections. Here, an analysis about the methods, results and what they are suggesting is addressed to state the final remarks of the presented research project. First, we present a discussion that sums up the results obtained and establish links between them. Then, the main conclusions of the research project are drawn pointing this work's novelty. Finally, the outlook for future research is presented to establish a possible path to continue research within this field of knowledge.

6.1. Discussion

The HF modeling approach consists of three models that use different input data, governing expressions and numerical solutions to study how water flows within porous beds under the effect of overlying flows, represented by boundary conditions, fully solved flows, or mathematical expressions that drive pore water flow in different directions. All of the three models are physically based and use expressions derived from the continuum mechanics to solve the proposed flow problem. The approach taken in each one of the three models allows this research to present novel findings in the area of Hyporheic Flow under different assumptions and conditions. One other thing these three models have in common is the scale or process based domain in which they are located: the hydrodynamics scale / ecological process based domain. Here, it is clear for all of the models that the main driving process is the change in pressure due to the hydrodynamics of the surface flow that conditions the groundwater flow.

For the case of the Burgers' Equation approach, the length scale spans over 60 *cm*, in the NSE is not bigger than a couple meters and for the case of the particle tracking domain, it can represent different length scales ranging from $O(10^{-2})$ *m* to $O(10^{-1})$ *m*. For the three cases mean processes can be well described (at least in one dimension or for one flow property). In the case of Burgers' Equation, we could demonstrate that HF is highly affected by pressure gradients, since it is the only physical quantity lacking in the expression that was used.

For the case of the NSE solved using OpenFOAM, the main takeaway is that it is possible to model HF as a single process with different conditions within the flow domain. And for the case of the particle tracking model it was possible to identify the main processes that control sediment deposition, namely flow path generated by free surface flow and groundwater inflow/outflow and filtration coefficient provided by the material from which the sand bed is made of. Some common flow features found in the proposed models are: (i) Greater flow velocities are always going to be found at the Sediment Water Interface and it will decrease with depth until reaching a constant value that can be safely assumed as Darcyan flow. (ii) There is turbulent flow in the porous media just below the free surface flow and as far as we know it can be averaged just as any other turbulent flow with different closure models. (iii) Processes in the ecological scale, driven by hydrodynamics will take place in the top part of the porous media, they do not tend to travel far down as shown by the three numerical experiments and their experimental counterparts. (iv) Continuous media is a feasible approximation for modeling Hyporheic Flow. However, not all of the physics can be represented due to the simplifications needed. Despite these four important findings, each one of the proposed models present strong and weak points that render it feasible to be used under different circumstances.

First of all, the three considered models do not take into account the effects of natural media such as moving bedforms or natural heterogeneous configurations. The closer our models get to represent heterogeneity is via mean physical features of natural media where flow is happening, i.e. porosity, permeability, hydraulic conductivity, among others. In second place, our models lack of validation in field. This means that the comparisons used during this research were performed with controlled experiments, either with controlled geometries or controlled dimensions and flowrates. Finally, but not less important, the way our models handle turbulence is not complete yet. For the case of the particle tracking model, for instance, turbulence effects are neglected and results lack of precision due to this failure. For the case of the NSE, the use of arbitrary constants for the coefficients hindered the quality of the results, but there was no information available on how to change those parameters (especially the apparent viscosity). And in the case of the Burgers Equation use, it is clear that the lack of pressure terms and mass conservation governing expression present a problem when modeling vertical velocities and consequently results and features that concern vertical velocity or stresses quantities are not useful at all. These factors sum up the models' limitations. However, research had also limitations that have to be pointed out.

In first place, the lack of data to compare and assess the models is a common shortcoming when talking about groundwater surface water interactions. In fact, scientific community efforts are trying to overcome this issue by creating a river database with different types of data in order to assess and evaluate models from different parts of the world. The second research limitation is the case dependency of the studies that have been found or used for referencing. As it is pointed by Ward and Packman (2019), there are lots of results from different places pointing even different evidence and contradictory results about the same phenomenon. This makes difficult sources of information picking and assessing results from the models built. Finally, the scale identification becomes a problem for the research, since none of the results obtained in this research can be extrapolated for several orders

of magnitude without having problems of consistency between model results and observed flows in field.

6.2. Conclusions

The results presented in the three previous chapters constitute the development of the the specific objectives proposed in the thesis proposal approved on 2016. A conceptual model that includes governing expressions for HF was set up via the Burgers' Equation, the use of the NS Equations and the APM, taking into account free surface and porous media flows (specific objective *i*). These conceptual models were implemented using three different numerical techniques, i.e. SMPM, Finite Volumes Method and Numerical Particle-Tracking with a Lagrangian approach. Therefore the numerical model proposed in objective number *ii* was met via these implementations. Furthermore, all of the results were compared by either qualitatively or quantitatively means with physical experiments, showing that these approximations are valid interpretations of Hyporheic Flow within the process domain continuum selected (specific objective *iii*). The presented models fostered our understanding of Hyporheic Flow and the processes that controlled, affected or disturbed it within the selected scale.

Going from a simple to a more complex approach, the Burgers' Equation was presented as a feasible model that took into account velocity dissipation between free surface and groundwater flow. Here, HF is modeled as a complex transport phenomena composed by a constant diffusive coefficient in the porous media and by the turbulent momentum exchange due to the local acceleration terms in the governing expression. The results suggest that this approach is valid in the streamwise direction as long as the free surface flow velocity field is captured with enough detail. Nonetheless, the weaknesses in modeling the vertical flow velocity and turbulent stresses suggest that the use of the Burgers' Equation as a proxy for Hyporheic Flow in granular beds leads to errors in vertical velocity profiles because of the assumption of hydrostatic pressure within the domain. Therefore, considering the use of a less precise scheme such as the Finite Volume Method, but including the pressure term of the Navier-Stokes Equations seems to be a more feasible solution to the problem of solving Hyporheic Flow.

Regarding the use of the Navier-Stokes Equations and the OpenFOAM package, results show that the velocity profiles as a whole are more coherent with experimental results. However, the change of numerical scheme brought less information. On other words, the NSE model implemented used mean turbulent equations, thus removing some detail from the solution proposed with the Burgers' Equation. However, modeling the whole process with pressures and velocities would make the model expensive in computation and time terms. Furthermore, the inclusion of apparent viscosity terms and/or drag terms to dissipate flow velocity appears to be more logical than the case of adding terms to the Burgers' Equation. Indeed, source/sink terms added to the momentum conservation equation of the NSE, makes more sense because of different average techniques such as the ones applied by Whitaker (1996), Breugem et al. (2006) and other authors, who include the "Forcheimer Tensor" to take into account the

stresses and flow opposition exerted by the porous media to the water flowing through it. The novel approach taken in the NS section was the modification of open source code to model two domains in a single model without having to impose boundary conditions to pass information between the free surface flow domain and the porous media.

The last model that put together this framework is the Particle-Tracking approach to model sediment deposition in sand beds using the Advective Pumping Model (APM). Despite being the simplest flow model for sand beds, the APM is widely used in fine sediment beds for its simplicity and good results in small scales case studies. In fact, for the case analyzed, the results suggested that fine sediment deposition depends on two factors: (i) the flow net within the domain and (ii) a filtration coefficient for the sand bed material used in the experiment. Although results are convincing and the comparison with real case studies is successful, the model lacks of implementing the effects of turbulence, hence all of the deposition patterns are not captured by the particle tracking framework. Future work on particle tracking includes models that take into account the interaction between the particles and the changes in permeability within the porous media due to the deposition of fine sediments.

To sum up, a modeling framework for Hyporheic Flow was presented for accomplishing the objectives of this research. A simple approach using a nonlinear transport equation (Burgers' Equation) to estimate velocity dissipation within porous media was analyzed at first; then, an application using commercial software (MATLABTM) and a low order scheme was used to solve the Navier-Stokes equations in a single domain but with different properties within it; finally, a particle-tracking approach was used to determine how fine sediment particles follow exactly the flow path described by streamlines and accumulate in determined places of a riverbed according to the velocity they have, while traveling through a flow path. Each one of the approaches states a specific form of approach to HF according to available data, scale requirements and/or tools available to model it. Despite those efforts, it is clear that a generalized Hyporheic Flow Hydrodynamics model is far from achieved and that efforts from all of the scientific community working in this topic have to be focused in the particularities of this phenomenon.

6.3. Outlook

The models used during this research project foster our understanding about Hyporheic Flow and Hydrodynamics of complex media. Nevertheless, their shortcomings show that each one of them can be improved adding physical properties that are not taken into account. On one hand, the NSE model shown in **Chapter 4** can be improved adding variable physical conditions in the simulated bed to take into account anisotropy and heterogeneity. On the other hand, the particle tracking model developed in **Chapter 5** can be improved by adding the feedback between sediment deposition and hydraulic conductivity, the effects of turbulence in the free surface flow and sediment deposition, and the inclusion of moving bed forms due to free surface flow. Nevertheless, the author does not recommend the use of the Burgers' Equation because of the results shown in this research project.

According to what our results suggest, numerical models based on classical fluid mechanics can be improved and implemented to further understand Hyporheic Flow and hydrodynamics of the Hyporheic Zone. The inclusion of more processes and interactions between sediment deposition, free surface flow, groundwater flow and reactive transport will help the understanding of the main research topic developed in this document. Specifically, if the upcoming results are to be implemented in Colombian Andean Rivers, numerical models should focus in porous media heterogeneity and clogging due to sediment transport.

Although flume models and numerical models in small scales are useful to understand HF, its drivers and effects; upscaling these processes to regional models is a task that has not been tackled yet. Results from different studies differ substantially and there is no consensus in the scientific community about fundamental processes and effects. To conclude, Hyporheic Flow and Hyporheic Exchange remain an open challenge for science nowadays. Results from this research project aiming to solve the specific problem of flow within the HZ make progress in the field but give no definite lights on the topic. However, our results suggest that Hyporheic Flow will be better understood continuing with a research path that consists of the following topics:

- Use of spectral methods to solve complex hydrodynamics problems focused in a single fluid flowing along different domains. This will bring faster and more precise solutions to flow and transport equations for Hyporheic Flow
- Modeling the effects of turbulence within porous media. Build models able that take into account turbulent and avoid the simple coupling of Darcy's Law and Navier-Stokes Equations
- Estimation of fine sediment deposition taking into account complex hydrodynamics, turbulence and moving bedforms
- Coupling hydrodynamics, sediment deposition and Hyporheic Exchange in different scales to assess the feedback between those three phenomena
- Integration between models and data in an iterative way to improve the knowledge of the Hyporheic Zone due to the lack of data, especially in riverbeds
- Use of flow models such as Multi Rate Mass Transfer to simulate different mean velocities in a single domain
- Physical experimentation aiming to estimate river bed properties and features under different flow and sediment deposition conditions
- Field measurements in small streams under strict protocols to be compared with existing data, avoiding by these means to generalize with insufficient data

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