Multi-Phase 1D Model for Particles and Constituents Transport in Tidal Systems

Doctoral Research Proposal

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September 2010

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Chapter One: Introduction and Motivation

1.1- Introduction

The numerical computation of the transport of constituents in river networks has become an essential tool for the planning, design, and assessment of the feasibility of water projects. Although the physical, chemical, and biological processes associated with the transport and fate of constituents in rivers have not yet been completely elucidated (see for instance, Massoudieh et al., 2010), engineers around the world are constantly called upon to provide answers regarding the exposure of animals and plants to contaminants, at diverse spatial and temporal scales. In this context, any development of computer simulating tools for the analysis of constituent transport in rivers should incorporate the most appropriate theoretical models to represent partially-understood, complex phenomena, and should adopt the most robust numerical techniques in order to provide optimized answers in practical cases.

One of the main technological motivations for this research is the analysis of sediment transport in the Sacramento-San Joaquin Delta, which is linked to the San Francisco Bay. These two water bodies form the largest estuary along the West Coast of the U.S. and have a notable importance for 25 million people in the California (Abiouli et al., 2007). There are many aspects in the Delta which are affected or impacted by sediment transport, namely: biological communities, levees, wetlands, construction of dams on major rivers, water diversion projects, dumping of urban and industrial waste in the bay, and dredging and navigability of waterways. There is a lack of validated tools for more precise analysis of the sediment transport in this estuarine system.

Seeking for and developing numerical tools for the sediment transport problem in the Delta, this writer found himself with clear scientific unanswered questions which are the scope of this Ph.D. proposal, as listed below as scientific motivation.

1.2- Scientific Motivation

This research focuses on the analysis of transport equations that include advection, diffusion, and reaction to solve most phenomena in environmental engineering. Sediment transport equations are one particular example of such ADR equations, but the outcomes of this research are applicable to other systems as well. The three processes (A, D, and R)

are highly variable in natural problems, from very reactive flows in groundwater pollution to highly advective flows in rivers. These ranges are characterized by two non-dimensional numbers: *Peclet* number which is defined as a measure of the relative dominance of advection versus diffusion, and *Damkohler* number which is the ratio of the reaction rate to the convection rate[i]. In this work, we solve the ADR equations with an Operator Splitting (OS) approach. OS has the following advantages over alternative methods:

a) The most appropriate discretization technique may be used for each process (it could be either implicit or explicit).

b) OS is capable of handling processes with different range of characteristic scales, in an efficient way by sub-cycling (sub-stepping) in one of the parts.

c) OS in practice is easier to employ in comparison with other equivalent methods.

d) Further modifications and developments are very straightforward in the OS schemes compared to the direct methods.

The goals of the present research are as follows:

Goal 1: Contribute to the understanding of the robustness, accuracy, and well-posedness of ADR solvers for the scales of environmental problems in rivers and estuaries, using Operator Splitting.

Goal 2: Contribute to the understanding of the phenomenon of infiltration of sand in gravel-bed streams without pattern recognition techniques in the measured data, and only by means of the constitutive physical laws.

1.3- Research Objectives

The first and second objectives are related to the first goal of the research and the third one addresses the second goal of the proposal.

Objective 1: Address the convergence and accuracy of a 1D, ADR solver based on Operator Splitting. Test those properties for different boundary conditions and varieties of operators' scales; Advection to Diffusion and Reaction to Advection.

Objective 2: Facilitate a reliable framework for verification of the accuracy and convergence of ADR solvers for environmental problems in the absence of analytical

[i] In some references the definition of Peclet and Damkohler numbers are the inverse of the above ratios.

solutions through the development of solution based on the*Method of Manufactured Solutions* (MMS).

Objective 3: Develop a theoretical/mathematical model for *gravitational infiltration of sand in gravel beds* in bed-load motion.

1.4- Technological Motivations

There are numerous issues which bring technological motivation to the present research proposal as follows:

- **Environmental Concerns:** Since the industrial revolution man has used estuaries and rivers to dispose of his waste. This has been the case since man first lived near rivers and estuaries, but pollutants were mainly organic and biodegradable. As populations expanded, geopolitical factors gathered people together in larger groups and people more often settled in the banks of rivers for many obvious reasons. With Industrial Revolution came the advent of toxic and dangerous chemicals as byproducts and the obvious place for these were in rivers and estuaries (Towner, 1994). Sediments have a major influence on the behavior of chemical constituents in estuaries. The high organic matter content in estuaries and the high biological productivity of sediment results in sediment exerting demand for dissolved oxygen from the overlaying waters (SOD[ii]). The deposition of nutrient rich organic detritus and its subsequent biological decomposition means that estuarine sediments act as both sink and source of nutrients such as phosphorous and nitrogen; sediment acts as a reservoir for nutrients (Chapra, 2008). In addition to their role in the nutrient and oxygen balance of estuaries, sediments are of critical importance due to their interaction with contaminants and introduced to rivers and water bodies by industrial activities. These contaminants may include trace metals and metalloids such as lead, zinc, copper, mercury, arsenic or selenium, and organic micro-pollutants, such as pesticides, petroleum hydrocarbons, and so forth. With large chemically reactive surface areas, sediments absorb and concentrate many of these pollutants from the water column and as a result estuarine sediments act as a major sink for pollutants introduced to estuaries (Forstner and Wittman, 1983). A major motivation for a tool to analysis of sediment movement pattern is; that can often provide a useful

[ii] Sediment oxygen demand

means of determining the degree of contamination of an estuary by pollutants (Forstner and Wittman, 1983). Even pollution histories of estuaries can be reconstructed by examining undisturbed dated sediments.

- **Climate Change Simulation:** The climate record over the last 100 years or so exhibits ample evidence for variations in rainfall, river flow, and mean sea water level (Jones et al., 1986), but we have little understanding of what causes and controls these regime changes (Karl, 1988; Wunsch, 1992). Understanding how climate variations will impact engineering facilities design and maintenance policy is an issue of increasing concern. Of particular interest are climate variations which occur within the facilities' lifespan. In the absence of rigorous predictive tools for future, researchers, by means of

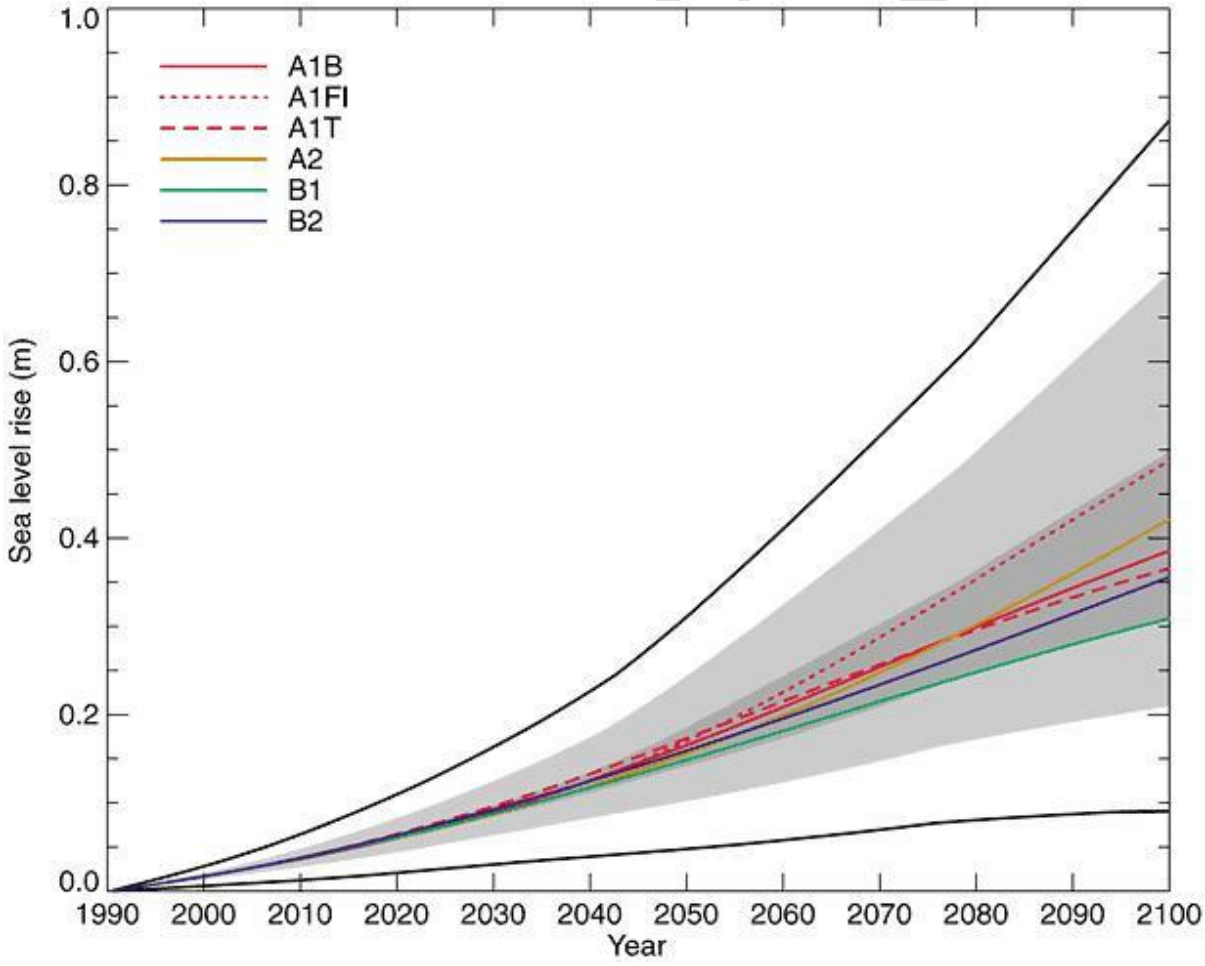

Figure 1: Sea level rise predictions forecasted by different scenarios for the next century (Intergovernmental Panel on Climate Change 2001)

stochastic models or by incorporating deterministic assumptions, have developed some probable scenarios for the Delta. The mentioned scenarios for the Delta outflow and

mean sea level (*MSL*) could be modeled by a sediment transport model to provide an overview of the long term picture of the Delta's morphological pattern. Sediment transport, likewise all other kinds of transport phenomena governed by advection, diffusion, and reaction of mass. ADR solver is the core engine in all sediment transport codes. Designing, planning, and maintenance of waterways, harbors, and water conveyance facilities could be modified based on the results of long term morphological vision of the Delta.

- **Bed Material Sorting:** Sediment engineering objectives that previously focused on erosion and sedimentation in engineering structures have been increasingly concerned with assessment of ecological indices and restoration design. While these studies often require classical computations of bed level or volume change, there is a growing interest in the evaluation of bed gradation transience in response to natural or anthropogenic events or planning alternatives. Invertebrate habitat, salmonoid spawning suitability and hyporheic flux are all functions of bed gradation (Gibson et al., 2010).
- **Waterway Navigability:** Dredging by definition means maintaining the safe navigation depth of a channel or harbor (PIANC, 2006). Dredging plant is expensive to build and operate. A small trailing suction dredger may cost in excess of £ 1,000,000 (at 1989 value) and the useful working life of the plant will be between 10 and 30 years. The old definition of dredging would be the act of deepening in an area with the aid of a dredger. However there are a number of complementary activities which would reduce or even eliminate the need to dredge, such as flood control, implementing sediment traps, leveling the bed etc. Waterway designers can incorporate a sediment transport model as an interpretive tool for determining the source of sediment load in the Delta channels under different circumstances. In addition it could be used as a predictive tool to determine waterway equilibrium condition after carrying out an engineering project.
- **Engineering Design of Water Intake Facilities:** Rivers provide fresh water for urban and industrial consumptions in the Sacramento-San Joaquin Delta. The water intake facilities are able to work in a predefined range of total suspended solid (TSS). The working range is due to the design of their water treatment plant or other technical considerations. Numerical sediment transport simulation could be adopted for operation rule base of any water intake in the Delta. In addition the positioning of inlet

and plant settling basin can be located based on the sediment transport model's simulations.

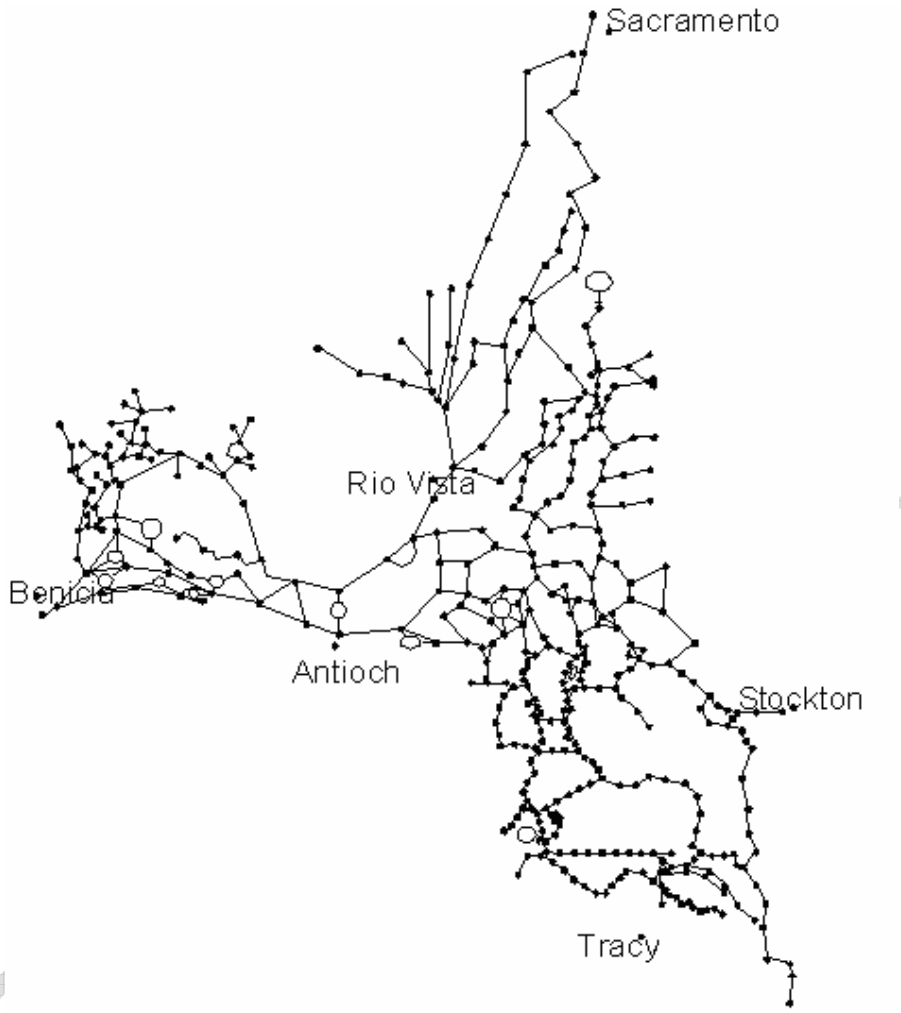

Figure 2: DSM2-Hydro, the Hydrodynamic Engine of the ADR Solver; Schematic of the Sacramento - San Joaquin Delta Grid. DWR Bay Delta Office, 22nd annual report (2001)

- **Boundary Conditions for Higher Dimension Local Models:** There is always a trade off between the details a model can provide and its computational costs. In recent decades there has been enormous progress in both efficient numerical schemes and computing platforms; however long-term 3D modeling of outsized domains is still not feasible even with adaptive meshes and other novel methods, due to shortcomings in computational resources. On the other side, for simulating phenomena such as local scour, breach processes, flow and sediment patterns in an intake, 3D modeling is the last resort before the expensive physical modeling. There is a middle way for addressing the above

problems; implementing the 3D model in the location of interest and expanding the domains to attenuate the BC-imposed error. After a certain limit the BC could be provided with 1D code without practical drop in the accuracy. The sediment transport model could be incorporated for coupling with more detailed codes, and providing the BC for their simulation domain.

- **Application to Conflict Resolution:** In the Sacramento-San Joaquin Delta there are many marinas and harbor facilities. Maintaining the facilities due to the sediment problem is a costly practice. Some of the stakeholders claim the problem is due to others' activities. A quantitative sediment transport tool could help to quantify the claims and can be a base for conflict resolution.

Chapter Two: Knowledge Gaps and Methods

In this chapter the unanswered aspects in the sediment transport literature are briefly mentioned and the approach to address them is discussed.

2.1- Objective One: ADR Efficiency Improvement for Tidal Systems

In the literature of numerical methods for coupling source terms and transport by advection and diffusion, Operator Splitting became a classic method in the last two decades. Fractal step method or Operator Splitting (OS) has been used widely in geohydrology, chemical engineering, air pollution, and atmospheric simulation (Valocchi and Malmstead, 1992; Steefel and MacQuarrie, 1996; Sommeijer et al., 1981; Khan and Liu, 1995; Kaluarachchi and Morshed, 1995). There is also research in estuarine modeling with Operator Splitting. In one study, only the advection and diffusion processes were considered (Aiyesimoju and Sobey, 1989). None of the above researches rigorously used a 2nd order accurate splitting method. It is worth mentioning regarding the OS method that many conventional methods of solving ADR could be recast mathematically as operator splitting forms and vice versa (see Leveque, 2002). The direct Operator Splitting (Godunov Splitting) will produce 1st order accuracy in general unless the operators commute. The alternating OS (Strang, 1968) will produce general 2nd order accurate method. The proofs of the above statements were carried out by Leveque (1981) using *Fourier Error Analysis* and by Lanser and Verwer (1989) in the context of *Lie Operator*. That is worth mentioning; in the most general form, the equations of hydrodynamics and transport have to solve together but in nearly all of riverine and estuarine codes the OS employed and the hydrodynamic runs first then it feeds the transport solver.

Note: Some terminology is used in this proposal that may require explanation. Here the terms *Source* and *Reaction* are used alternatively in the mathematical context for all kinds of *sinks*, *sources*, *lateral inflows* and *chemical reactions*, or in general, the right hand side of the equation 1, that is our interest, as follows:

$$\frac{\partial(AC)}{\partial t}+\frac{\partial(AUC)}{\partial x}-\frac{\partial}{\partial x}\left(AK\frac{\partial C}{\partial x}\right)=E-D+q_{lat}+Sources-Sinks \qquad (1)$$

in which A is area [L^2], C is the constituent's concentration [L^3/L^3], t is time [T], x is streamwise direction [L], K is dispersion coefficient [L^2/T], E is entrainment [L^2/T], D is deposition [L^2/T], and q_{lat} is the lateral inflow of the constituent [L^2/T].

This terminology has been adopted from the works by Leveque (2002), Lanser (1989), and Sommeijor (1981), so the term *reaction* or *source* imply terms in the right hand side of equation 1, and does not mean *chemical reaction* unless it is mentioned in the text. We use the term *chemistry* for *chemical reaction*.

The entire *source terms* in this proposal are assumed to be *kinetically controlled reactions*. In this kind of reaction, the characteristic time scale is in same orders of the hydrodynamic characteristic time. In case they are assumed to be *instantaneous equilibrium reactions*, the text denotes them as *instantaneous reactions*. Treatment of instantaneous chemical reaction in general needs and implicit solver and the source term in this kind of phenomenon should solve simultaneously with other interacting constituents.

The sediment source term of entrainment and deposition functions for non-cohesive sediment transport phenomenon is provided in the appendix C-1 and the relations for cohesive sediment transport is attached in the appendix C-4 of this proposal.

Second-order accurate operator splitting

Consider the following IBVP[iii]:

$$\frac{\partial u}{\partial t} + Lu = 0 \qquad in\ (0,T)\ ,\ u(0) = u_0 \tag{2}$$

(Strang splitting[iv]) $L = L_1 + L_2$ (3)

$$\frac{\partial u}{\partial t} + L_1 u = 0 \qquad in\ (t^n, t^{n+1/2})\ ,\ u(t^n) = u^n \rightarrow \tilde{u}^{n+1/2} = u(t^{n+1/2}) \tag{4}$$

$$\frac{\partial u}{\partial t} + L_2 u = 0 \qquad in\ (t^n, t^{n+1})\ ,\ u(t^n) = \tilde{u}^{n+1/2} \rightarrow \tilde{\tilde{u}}^{n+1/2} = u(t^{n+1}) \tag{5}$$

$$\frac{\partial u}{\partial t} + L_1 u = 0 \qquad in\ (t^{n+1/2}, t^{n+1})\ ,\ u(t^{n+1/2}) = \tilde{\tilde{u}}^{n+1/2} \rightarrow u^{n+1/2} = u(t^{n+1}) \tag{6}$$

The greatest difficulty with Operator Splitting arises in defining the intermediate boundary conditions of the equations (5) and (6). Theoretical developments of the

[iii] Initial Boundary Value Problem

[iv] The decomposition of L is non-unique $L = L_1 + L_2 + L_3 = L_1' + L_2'$, also the operators can be grouped in different ways $L_1 + L_2 = L_1'$, $L_3 = L_2'$ or $L_1 = L_1'$, $L_2 + L_3 = L_2'$

intermediate boundary condition have been presented by Leveque (1983), Aiyesimoju and Sobey (1989), Sommijier et al. (1981), Khan and Liu (1995) for two operators (reaction was not included) or case of *Godunov* Splitting (1st order accurate). The development of 2nd order accurate approximation of the intermediate boundary condition for three consecutive operators (Advection, Diffusion and Reaction) could not be found in the literature to the best of my knowledge and afford a good opportunity for research.

The question here is: do we really need high resolution OS method? Maybe the low resolution schemes could be employed for small domains or short time spans, but in the historical runs and oversized domains accumulation of error will ruin the results. On the other hand the refinement of the mesh is not always feasible due to the limitation of computational resources. Thus, undoubtedly a high resolution solver is required for dealing with an oversize IBVP problem. To have a quantitative picture from the BC imposed problem, compare the L_1 values in the tables 11 with table 12, first case is Godunov splitting with trial exact boundary condition and the second one is the same problem which is subjected to zero order non-trivial boundary condition, In the former convergence ratio is approximately *1.95* and in the latter it drops to *1.02*[v], solution accuracy is also drops *2* to *3* order of magnitude as well[vi].

In this research, the equation of interest is equation (1), the details of erosion and deposition could be found in appendix *C*. The first aim is determining the error caused by operator splitting. This error will be calculated by defining a very large domain, run the problem, and calculating the error norms, and calculating mass for an ADR benchmark case which is subjected to trivial zero flux boundaries at far left and right of the domain. In the next step, the zero order, first order and second order approximations of the boundary condition will be derived for ADR splitting. The effect on accuracy and order of error convergence will be studied for different splitting methods (Godunov and Strang), boundary condition implementation (zero, first, and second order) and different ranges of dimensionless numbers (Peclet and Damkohler).

[v] In OS, Splitting error is a function of commuting of operators (Sommeijer et al. 1981), since in all of the previous researches the study were conducted based on comparing with the analytical solutions in which the Area, Velocity and Dispersion coefficient are assumed to be constant, the author expects even larger error in case of non constant coefficients.

[vi] Both problem where observed in the same portion of domain.

If an equal portion in the middle with the same grid size is assumed (labeled by *Observation Part* in figures 3 and 4), and the same problem as first part (the part with trivial correct boundary condition) is considered, we may distinguish the error due to the boundary condition in operator splitting.

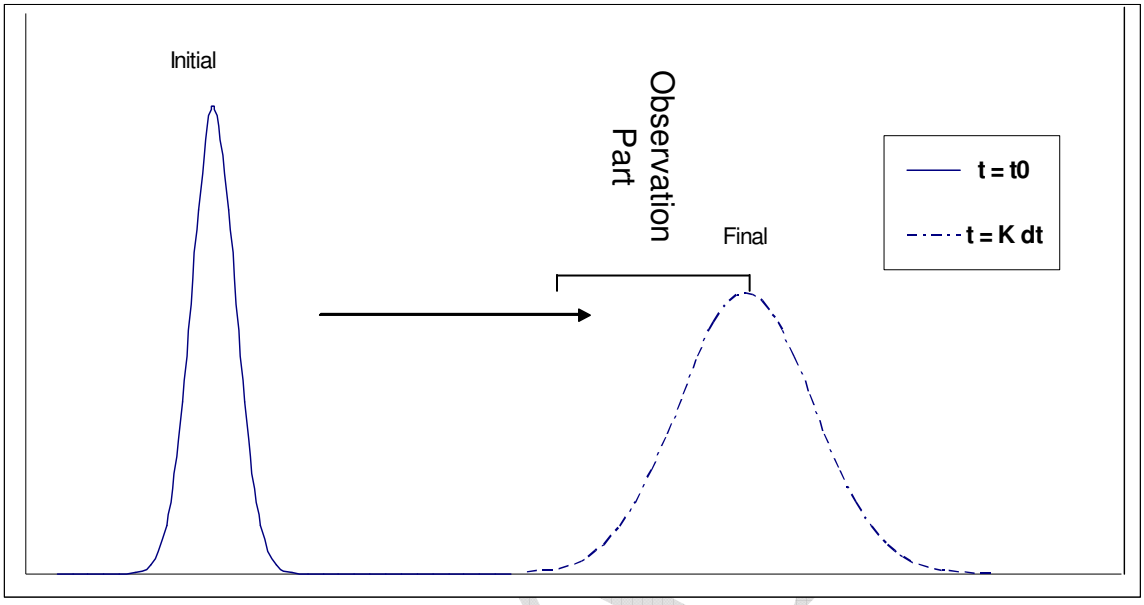

Figure 3: Schematic of a domain with trivial zero flux boundary

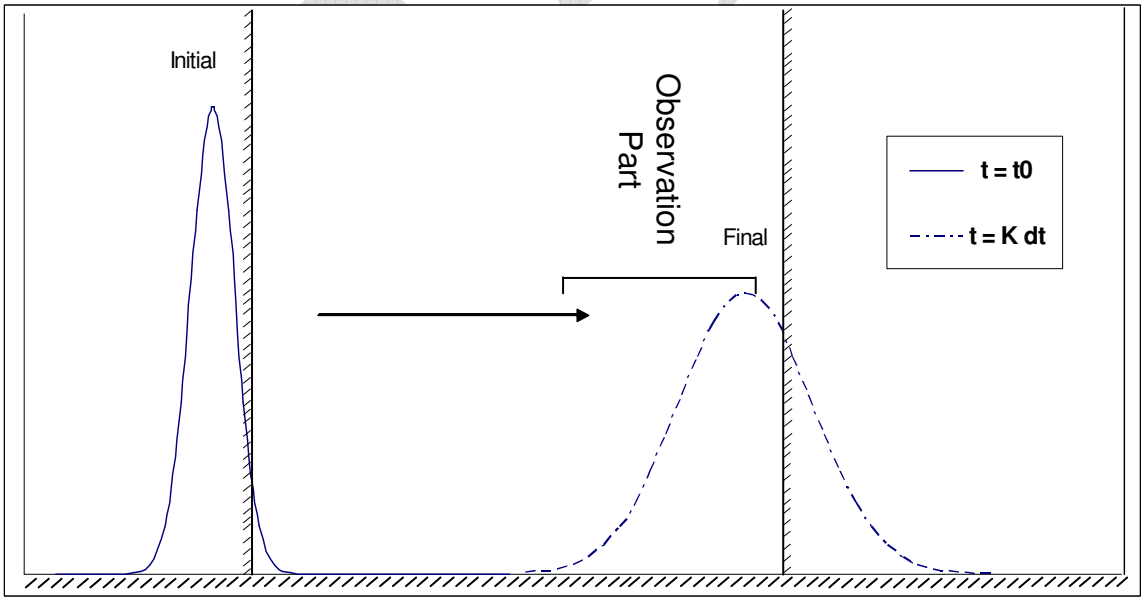

Figure 4: Schematic of a domain with non-trivial boundaries to study effect of different boundary conditions on accuracy and error convergence rate.

One of the knowledge gaps in the OS literature which is going to be addressed here is the study of convergence rate behavior with different intermediate boundary conditions. The

other original deliverable of this research will be the study of the accuracy of the OS solvers based on different ranges of the dimensionless numbers.

2.2- Objective Two: Rigorous Verification of the ADR Solver

The general form of ADR equation which was our interest in *Objective 1* is:

$$\frac{\partial\left(A(x,t)C(x,t)\right)}{\partial t}+\frac{\partial\left(A(x,t)C(x,t)u(x,t)\right)}{\partial x}=\frac{\partial}{\partial x}\left(A(x,t)K(x,t)\frac{\partial C(x,t)}{\partial x}\right)+R\left(u(x,t),C(x,t)\right) \quad (7)$$

where A is Area, C is concentration, u is velocity, K is longitudinal dispersion coefficient, and R is the source term. The question here is: if one wants to find accuracy and convergence ratio of a scheme in which the analytical solution is unknown (absence of analytical solution is the main motivator towards all numerical methods), what should be done? It is ideal to test a model's correctness by comparing its numerical results with analytical solutions; however the difficulty is that there is not a general solution for the non-linear IBVP in hydrodynamics. There are some ways to deal with this problem: *Richardson Extrapolation* in the applicable situations (Roache and Knupp, 1993), comparison of results with another higher order solver (the benchmark solver must be verified beforehand), we can reduce the mesh size and compare with in relative terms, *Method of Manufactured Solutions* (MMS), and *Prescribed Solution Forcing Method* (PSF) (Wang and Jia, 2009). The basic concept of the MMS and PSF is to compare the correctness of numerical solvers using an arbitrary manufactured function. MMS and PSF are conceptually following the same idea, although the former is more general than the latter. PSF have been used for the verification cases in which the user can not access the source code to define boundary conditions like some groundwater codes. Since the author with his code, is able to define the boundaries, the objective *2* will be carried out through MMS.

The Method of Manufactured Solutions is a general approach to provide a certain analytical solution of the governing equation for the question of model testing and verification of non-linear numerical solvers in rigorous procedure. Since only the numerical method is to be tested (not the physics of the problem) it would be effective if an arbitrarily made non-linear function can be used in model verification. The exact solution which is manufactured in this method does not need necessarily be realistic

(Roache 2009, 2002; Wang et al., 2009) because the verification is a purely mathematical process. We want a benchmark solution that is non-trivial but analytical, and that exercises all ordered derivatives in the error expansion and in all terms.

Let the differential equation be expressed as:

$$L(u) = 0 \tag{8}$$

in which L denotes the differential operators and u is the variable to be solved. When a manufactured function φ is substituted into the differential equation, one would have:

$$L(\varphi) = R \tag{9}$$

Since φ is not the solution of differential equation, the non-zero R is obtained analytically. In the solver, the numerical solution of this equation would be forced to converge to φ with the analytical forcing term R being added to the mathematical equation of the numerical model as the source term. The verification of a numerical model is simple because the solution of equation (7) is known; one needs only compare the difference between the manufactured analytical function, φ, and the numerical solution of equation (7). Although the function φ can be manufactured arbitrarily, it has to be non-trivial for all the terms of the involved mathematic equations to make a meaningful verification tests. MMS does not require the satisfaction of any particular boundary condition other than those defined by φ along the boundaries of computational domain. The following example clarifies the method:

Example 1: Development of a MMS for Eq.(1) (Zamani et al. 2010)

Since the MMS ends up to a source term, we may assume the simplified ADR governing equation as (10) which initially does not have source term:

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(AUC)}{\partial x} = \frac{\partial}{\partial x}\left(AK\frac{\partial C}{\partial x} \right) \tag{10}$$

$$\begin{cases} c = c(x,t) \\ x \in (0,\ 1) \\ A(x,t) = 100 - 15x + 20\sin(\omega t) \text{ --->} \ \ 65 < A(x,t) < 120 \\ K(x,t) = 3 + \sin(\pi x) + \sin(2\omega t) \text{ --->} 1 < K(x,t) < 5 \\ U(x,t) = 1 + 2\cos(\pi x)\sin(\omega t) \text{ --->} \ -1 < U(x,t) < 3 \end{cases}$$

There is no restriction on the boundary and initial condition, they will be appear automatically after choosing the function for manufactured solution.

$$L(C)=\frac{\partial(AC)}{\partial t}+\frac{\partial(AUC)}{\partial x}-\frac{\partial}{\partial x}\left(AK\frac{\partial C}{\partial x}\right)=0 \tag{11}$$

The above is governing equation in a very general form (area, velocity and dispersion coefficient are spatial and temporal variable), since the method is a general concept, any solution for C can be picked regardless of the governing equation, so we pick the (12) and insert it in to the (11):

$$\tilde{C}(x,t)=x^{2/5}(2+Sin(t)) \tag{12}$$

The function which is picked for MMS must not vanish in the governing equation, so for advection and diffusion, C must be at least from C^1 space in x domain and C^0 space in time domain (the C in Eq. (12) is always smooth or belongs to C^∞ space).

$$R(x,t)=L(\tilde{C})$$

$$\begin{aligned}R(x,t)=&-15(2+\sin t)(x^{2/5})(1+2\cos(\pi x)\sin(\omega t))\\&+\tfrac{2}{5}(100-15x+20\sin(\omega t))(2+\sin t)x^{-3/5}(1+2\cos(\pi x)\sin(\omega t))\\&-2(100-15x+20\sin(\omega t))(2+\sin t)x^{\frac{2}{5}}\sin(\pi x)\pi\sin(\omega t)\\&+20\cos(\omega t)\omega(2+\sin t)x^{\frac{2}{5}}\\&+(100-15x+20\sin(\omega t))(\cos t)x^{\frac{2}{5}}\\&+6(3+\sin(\pi x)+\sin(2\omega t))(2+\sin t)x^{\frac{-3}{5}}\\&-\frac{2}{5}(100-15x+20\sin(\omega t))\cos(\pi x)\pi(2+\sin t)x^{\frac{-3}{5}}\\&+\frac{6}{25}(100-15x+20\sin(\omega t))(3+\sin(\pi x)+\sin(2\omega t))(2+\sin t)x^{\frac{-8}{5}}\end{aligned} \tag{13}$$

So the modified equation (11) is:

$$L(C)=\frac{\partial(AC)}{\partial t}+\frac{\partial(AUC)}{\partial x}-\frac{\partial}{\partial x}\left(AK\frac{\partial C}{\partial x}\right)=R(x,t) \tag{14}$$

Subjected to the initial condition:

$$\tilde{C}(x,0)=x^{2/5}(2+Sin(0))=2x^{2/5} \tag{15}$$

And the Neumann boundary conditions:

$$\frac{\partial\tilde{C}(0,t)}{\partial x}=\frac{2}{5}(2+\sin t)x^{\frac{-3}{5}}=0 \tag{16-a}$$

$$\frac{\partial \tilde{C}(1,t)}{\partial x} = \frac{2}{5}(2+\sin t)x^{\frac{-3}{5}} = \frac{2}{5}(2+\sin t) \qquad (16\text{-b})$$

Although the above algorithm seems straightforward at the first glance, the author faced practical restrictions as follows:

1. The ADR solver is only working in the feasible ranges of dimensionless numbers ($Pe = \frac{A_{Scale}}{D_{Scale}}, Da = \frac{R_{Scale}}{A_{Scale}\ or\ D_{Scale}}$) so in case the reaction rate in equation (7) is exceeds a certain limit, the ADR solver is not really tested on the nature of the physical problem.
2. Some of the coefficients in equation (7) can not have negative values (Area, Concentration and Dispersion Coefficient), and we prefer to check them in the scales which usually occur in nature.
3. Area and velocity must fulfill the continuity equation. So we can just set one of them and the other one is not our choice.

Therefore, finding the manufactured solution with these restrictions is not straightforward. The method to overcome the above restrictions is a novel method and to the best of the author's knowledge no one mentioned it in the literature yet. The idea is to start from a known analytical solution by Zoppou and Knight (1997)[vii]. We may perturb the answer, then insert the perturbed answer into the equation (10) to get the source term. The trick implicitly preserves the above mentioned restrictions. The symbolic math solver is incorporated to derive the equations and it will be called by FORTRAN code or hardwired in the FORTRAN source routine.

2.3- Objective Three: Model for Sand Infiltration in Gravel Bed

Although some people believe that the present time the theoretical methods dealing with ADR solvers are mature after nearly four decades of challenging the problem, the Achilles' heel in the modeling of constituent in general and especially sediment transport is the definition of the source term (Leveque, 2002; Ateljevich, 2010). The definition of erosion and deposition in sediment transport literature is based on empirical relations. Mehta and McAnally (2007) mentioned that the state of current

[vii] Appendix B.

knowledge is very far from being able to capture all the behavior of sediment erosion and deposition just by the constitutive laws in near decades. The attempts to derive a mathematical model of deposition based on a simplified model in *Pseudo-Lagrangian* framework will be addressed in this research. The problem of deposition here is reduced to deposition of non-cohesive sediment in a streambed with coarser material.

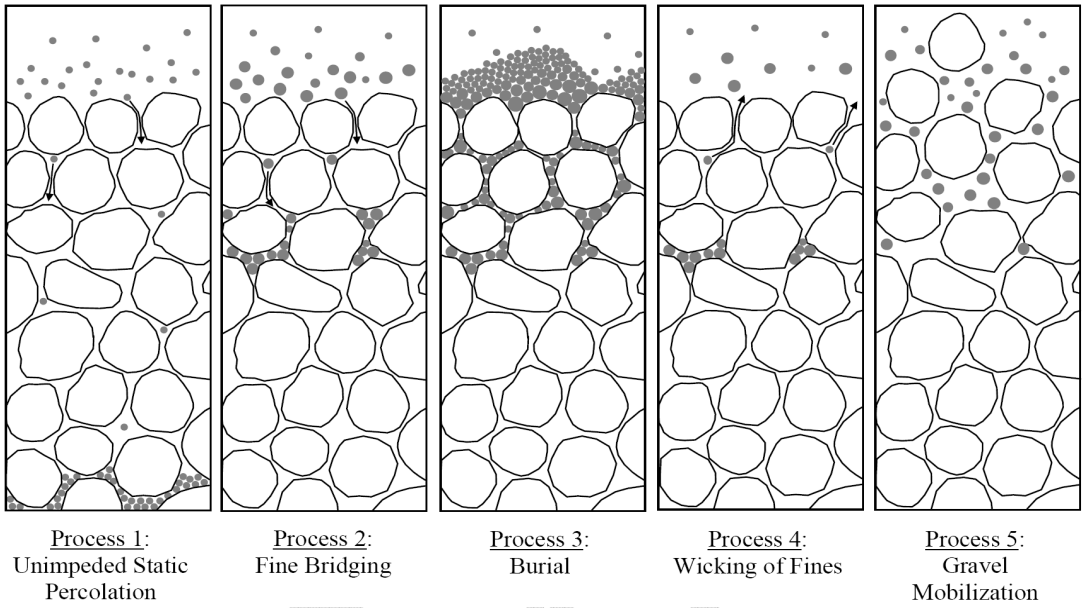

Figure 5: Schematics of Different Bed Fining Procedure (Gibson et al., 2009).

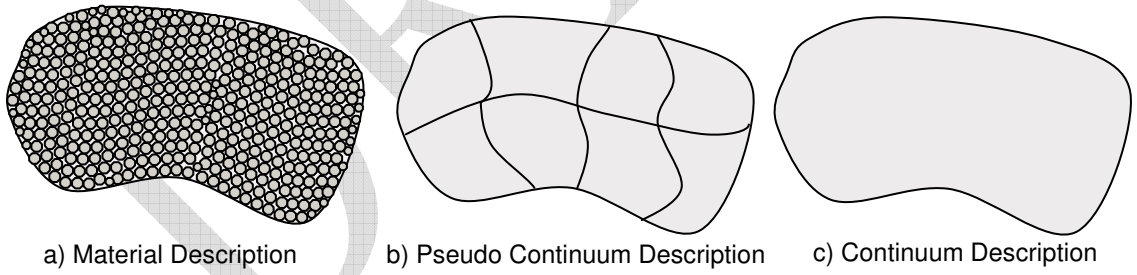

Figure 6: Different Frameworks for Description of the Sand Infiltration Problem

a)Lagrangian $M = \sum_{i=1}^{n-Particle} m_i$, b) Pseudo Lagrangian $M = \sum_{i=1}^{8} M_i$, c) Eulerian $M = \int dm$

Simplified Problem

Let's assume the distribution of material in all layers and the top sand layer in figure 7 are known at the beginning. For the sake of simplicity we just consider a 1D phenomenon (vertical). The problem could be approached in three different ways:

1- *Lagrangian approach* (figure 6-a); the infiltration process is a Markov Chain, the process at time *n+1* is only dependent of the system's state at time *n*. Individual sand parcels are traced until the time they trap in a layer and the porosity of the layer, has to be updated for new particles' combination, But there are clearly certain drawback: the number of parcels can be very large and computation becomes extremely costly.
2- *Pseudo Continuum*[viii] *approach* (figure 6-b); Same as above process, but the sand mass is divided to the smaller continuum subdivisions and at each time step, one portion is added to the layers beneath, then the porosity of layers is updated based on new particle combination in each layer.
3- *Eulerian approach* (figure 6-c); the mass is assumed to be continuum and the governing partial differential equation for time evolution of the porosity as a function of entered mass must be solved for each class. The problem here is: how to find the governing PDE of the problem?

Approach:

If we can derive the "void size distribution" and represent it by $\bar{d}$ at each layer, we will estimate how many void sizes the sand particle d' will have to cross, until it finds a $\bar{d}$ such that $\bar{d} < d'$. If it is assumed that in each step the particle moves a certain distance (a layer in figure 7), the mathematical procedure could be assumed as follows:

From discretization of grain size distribution of each layer into *m* classes we assume each class is represented by its average diameter, d_i; for each class of diameter the cumulative percentage F_i will be associated with a probability function P_i , and then with each d_i a probability of occurrence P_i will be associated. For example, let's assume we have a mass of sand on the top of gravel material. Here we just solve for the arrangement of three neighboring particles, in a bed which is made of three different particle sizes, but the procedure could be carried out for any arbitrary arrangement of particles and number of particle sizes.

[viii] In the literature of Atmospheric Science, this approach is called "Semi-Lagrangian"

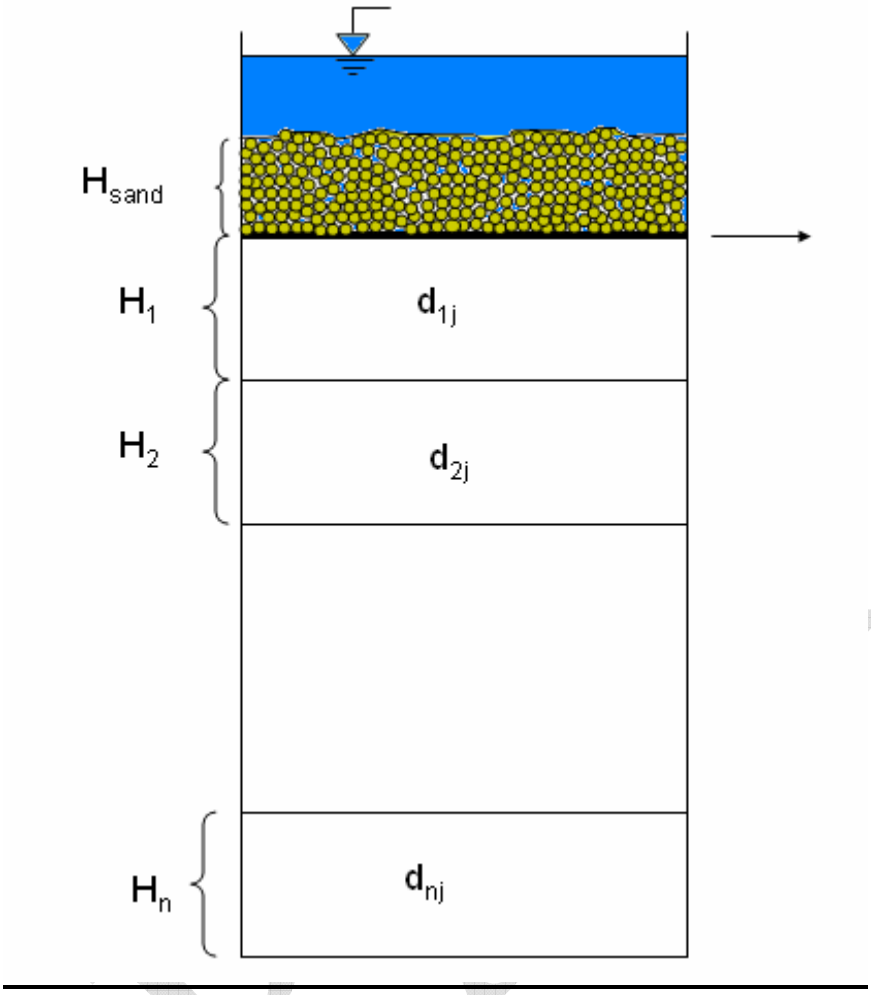

Figure 7: Schematic of the 1D gravitational sand infiltration problem

Three fundamental hypotheses will be established:

1- The river bed is at its maximum density[ix]
2- Particles are spherical
3- The relative positions occupied by the grains are random

In so doing it could be assumed that any point in the middle of the bed materials is made up of a three tangent spheres with diameters, d_k, d_l, and d_m and with corresponding probabilities P_k, P_l, and P_m that can be represented by the internal tangent circle of $\overline{d}$:

$$\overline{d} = f(d_k, d_l, d_m) \qquad (16)$$

[ix] It will be expanded in to loose bed material in further steps, with the void ratio between four and more adjacent particles, but the solution procedure is the same as above.

And we may compute the probability of $\bar{d}$ occurrence, $\bar{P}$ based on P_k, P_l, and P_m (Kemeny et al., 1959)

$$\bar{P} = \frac{3!}{r_k!r_l!r_m!}.P_k^{r_k}.P_l^{r_l}.P_m^{r_m} \qquad (17)$$

In which the r_q are the number of times that d_q occurs in a group and $\sum_{i=1}^{3} r_i = 3$ and r_i must be a non-negative integer number. Based on the $\bar{P}$, probability of entrance will determined and then the grain distribution updates, the whole procedure is repeated for the updated grain distribution until the difference between two successive steps converges to negligible value. The following example makes the procedure clear:

Example 2:

Let's assume we have 3 different sizes in the bed materials d_1, d_2, and d_3. In the sediment transport gravel and sand (non-cohesive sediments) can divided to *10* different sizes[x], and let's assume bed material is compact and the void paths are just through arrangements of 3 particles, *25%* of the grains are d_1, *35%* d_2, and *40%* d_3 [xi], all the permutations of bed particles are ten cases as follows:

$$\binom{3}{3} = 1: \; d_1 d_2 d_3$$

$$\binom{3}{1}\binom{2}{1} = 6: \; d_1 d_2 d_2,\, d_1 d_3 d_3,\, d_3 d_2 d_2,\, d_3 d_1 d_1,\, d_2 d_3 d_3,\, d_2 d_1 d_1$$

$$\binom{3}{1} = 3: \; d_3 d_3 d_3,\, d_2 d_2 d_2,\, d_1 d_1 d_1$$

In general, the total number of permutations of adjacent spheres is $C_m^n = \frac{(n+m-1)!}{m!(n-1)!}$, where n is total number of grain classes and m is the number of particles in each arrangement (three or four based on Frostick et al., 1984) so for *n=10,* and *m=4* we will have 2860 different arrangements. If we assume $d_1, d_2, d_3 = 10, 20, 40\,mm$, $\bar{d}$ the diameter of sphere which fits in the middle of d_1, d_2 and d_3 is calculated based on equation (18):

[x] From the limit of flocculation possibility, or very fine sand d>0.0625 *mm* to very coarse gravel d>32 *mm* by the ratio 1:2:4:8….

[xi] The layer material percentage could be defined based on number, area, or volume(mass) of grains

$$((d_1 + d_2 + d_3)d_1 d_2 d_3)^{\frac{1}{2}} = \qquad (18)$$

$$((d_1 + d_2 + \bar{d})d_1 d_2 \bar{d})^{\frac{1}{2}} + ((d_1 + \bar{d} + d_3)d_1 \bar{d}\, d_3)^{\frac{1}{2}} + ((\bar{d} + d_2 + d_3)\bar{d}\, d_2 d_3)^{\frac{1}{2}}$$

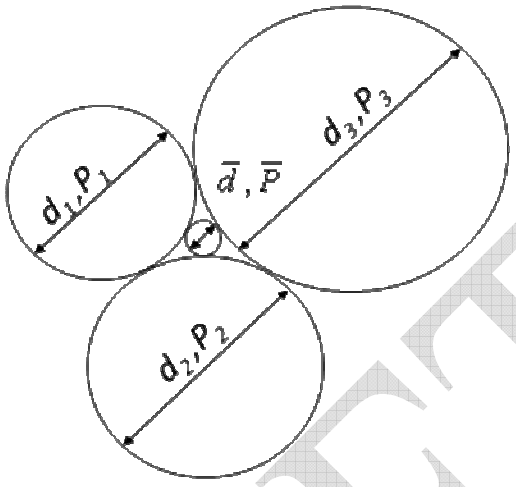

Figure 8: Filter Particles' Arrangment in Densest State

Each $\bar{d}$ will appear with probability $\bar{P}$, which is the probability of occurrence of the group (d_k, d_l, d_m) and by "*independent trial process*" in probability theory as defined by equation (17).

Table 1:calculation of void size distribution base on grain size distribution

Group	$\bar{d}$ (mm)	$\bar{P}$	$\bar{P}$	Cumulative void ratio %
$d_1 d_1 d_1$	1.55	p_1^3	0.015625	1.5625
$d_1 d_1 d_2$	1.9	$3p_1^2 p_2$	0.065625	8.125
$d_1 d_1 d_3$	2.2	$3p_1^2 p_3$	0.075	15.625
$d_1 d_2 d_2$	2.35	$3p_1 p_2^2$	0.091875	24.8125
$d_1 d_2 d_3$	2.75	$p_1 p_2 p_3$	0.21	45.8125
$d_2 d_2 d_2$	3.1	p_2^3	0.042875	50.1
$d_1 d_3 d_3$	3.35	$3p_1 p_3^2$	0.12	62.1
$d_3 d_2 d_2$	3.8	$3p_3 p_2^2$	0.147	76.8
$d_2 d_3 d_3$	4.7	$3p_1 p_2^2$	0.168	93.6
$d_3 d_3 d_3$	6.2	p_3^3	0.064	100
$d_1, d_2, d_3 = 10, 20, 40\, mm$ and $p_1, p_2, p_3 = 25, 35, 40\ \%$				

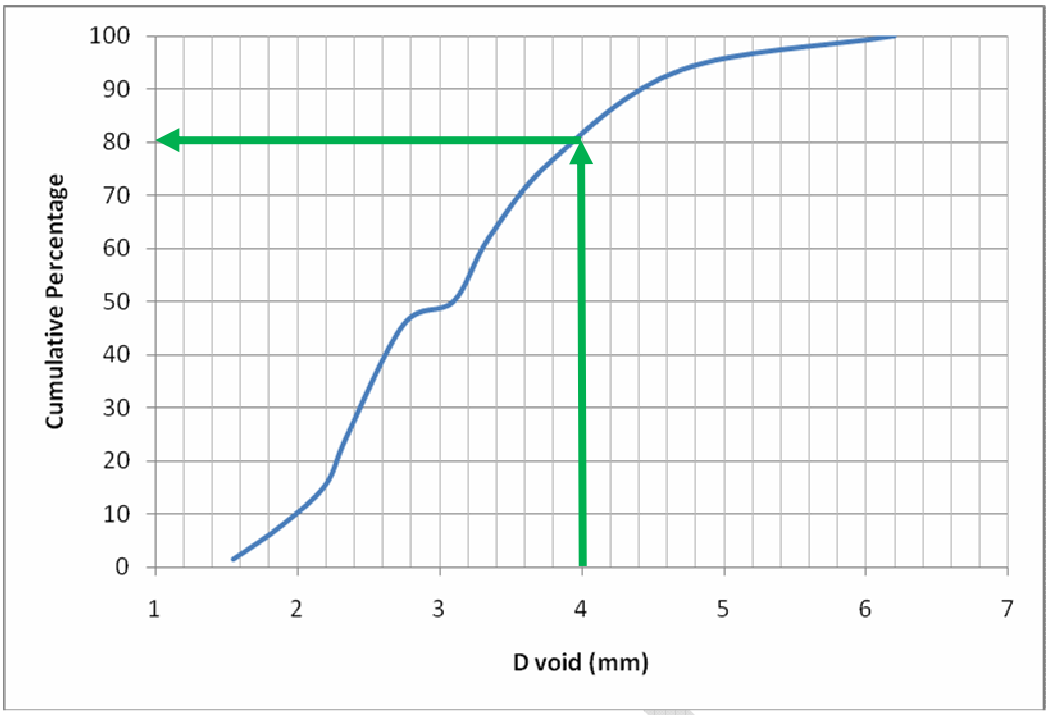

Figure 9: The void curve distribution for example 2

So if the sand size particle is smaller than *1.55 mm*, *100%* of it will pass layer one and if its size is larger than *6.2 mm*, it cannot penetrate the layer at all. Sizes between *1.55* and *6.2 mm* are able to enter the layer; at this stage we can let a portion of sand material enter the first layer, since we discretized the solution, and the portion of mass which is entered must be small compare to first layer's mass distribution (say *5%*). Some part of this sand will be trapped in the first layer and the remaining will penetrate into the second layer. If we can find the percentage which is trapped, we may update the layer's void curve distribution for the next iteration and continue the procedure until there is no meaningful change in the mass of each layer. For example for particle $d^*=4$ *mm* the percentage of confronting a void diameter greater that d^* is ($P=100-80=20\%$). Assuming that the encounters were carried out in an independent way, the probability that d^* will go in n proofs be P^n. Consequently, the probability that the particle d^* will be stopped after n proofs is $(1- P^n)$. If we assume a confidence level of P_c percent, that is, if we would like to have P_c percent of confidence that the particle will be stopped after n proofs we will have:

$$n = \frac{H_1}{\alpha d*} = \log\left(\frac{1-P_c}{P}\right) \qquad (19)$$

where α is a coefficient ($\alpha>1$) to make characteristic length to compare with layers thickness[xii]. The following flowchart briefly describes the approach to modeling the infiltration of sands in the coarser gravel bed-stream.

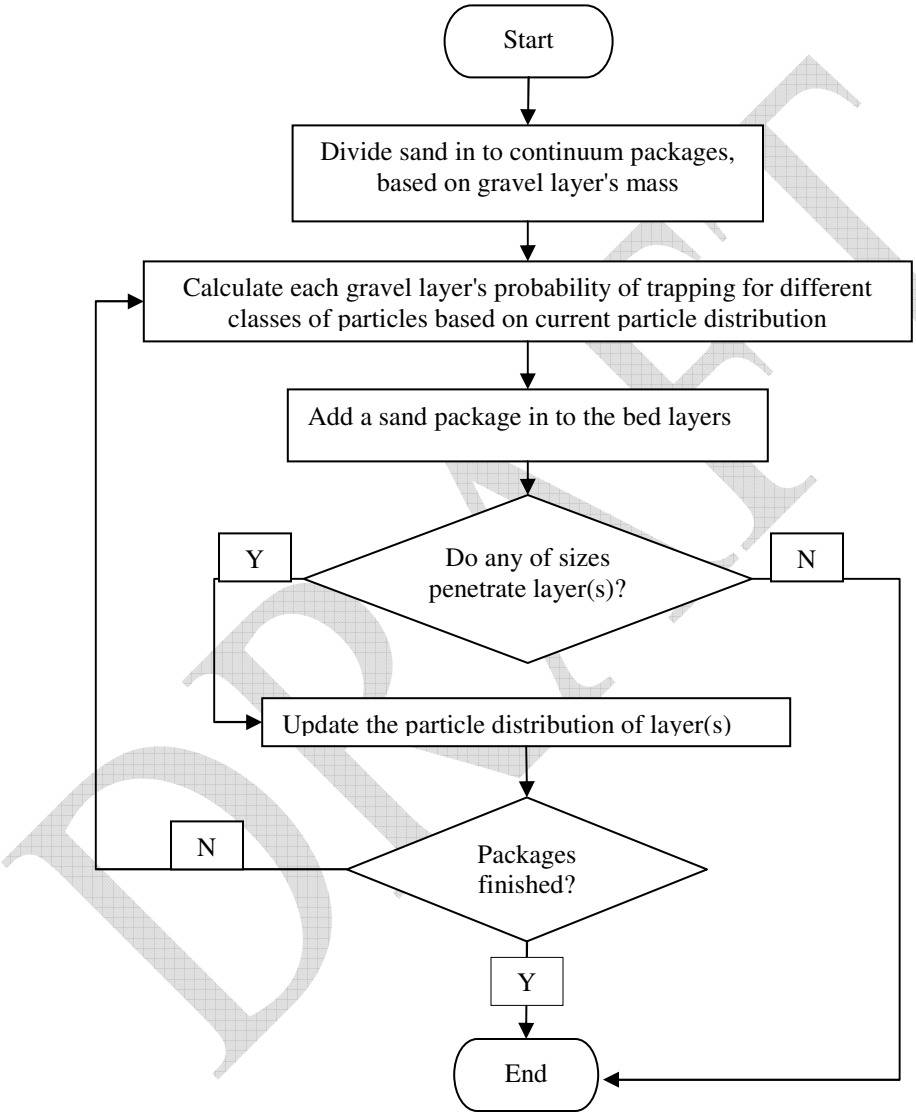

Figure 10: Schematic of the algorithm for modeling sand infiltration in gravel bed

[xii] It can assumed as the method's tuning factor

Chapter Three: Ongoing Work and Basic Results:

3-1. Testing Method

The style of coding is not only a vital issue in engineering practices and to deliver the correct results, but also it will be a crucial point in further modification in case of new theories, probable bugs, and expansions for additional capabilities. The ADR solver is coded with a professional plan adopted from software developing sciences:

1) Deriving the mathematical schemes and solution approach.

2) Design the coding in the modular structure.

3) The documentation of coding is written at the same time inside the code, and produces by a post compiler.

4) Writing the test unit for each individual unit in a mirror program which is designed for testing the ADR solver.

The ADR solver is coded in the most modular way. As a result further modification can be applied at lower cost. The unit test will run automatically every often and tests each unit and functionality so tracing a defect would be easier. Finally a post compiler (Doxygen) will go through the code and make a pdf document from the comments of the author inside the FORTRAN program. The rest of the document is dedicated to the results of the ADR unit testing package.

3-2. Advection

At the beginning the Advection solver was coded based on the Flux-based Modified Method of Characteristics (MMOC) (Roache 1992), but due to the practical issues of back tracing the foot of characteristic in high Courant numbers and junction of channels. we decided to choose an Eulerian approach: Modified Lax Two Step Method[xiii] (Leveque, 2002) with a van Leer MUSCL flux limiter (Saltzman, 1994; Arora and Roe, 1997). The details of discretization are provided in the appendix A-1. Advection solver is an explicit solver which is 2nd order accurate in both time and space.

[xiii] Detail of discretization in Appendix A-1.

Table 2: Test advection convergence subjected to tidal flow (Flux limiter off)

Number of nodes[xiv]	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	CFL= 0.39
256	1.022E-5	1.82E-6	2.683-4	2.805	3.22	2.75	Max Velocity = 0.43 m/s
128	7.146E-5	1.698E-5	1.804E-3				Flux Limiter is off
64	4.020E-4	1.263E-4	8.189E-3	2.49	2.89	2.18	BC Neumann Zero Flux

Table 3: Test advection convergence subjected to uniform flow (Flux limiter off)

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	CFL= 0.59
256	4.978E-6	6.03E-7	3.38E-5	2.99	3.49	2.98	Max Velocity = 1.11 m/s
128	3.95E-5	6.77E-6	2.66E-4				Flux Limiter is off
64	3.08E-4	7.41E-5	1.99E-3	2.96	3.45	2.90	BC Neumann Zero Flux

Since in sharp gradients flux limiter switch the gradient from higher order to lower order approximation, error convergence ratios drop -in not smooth problems- as a consequence of activating the flux limiter.

[xiv] In mesh refinement convergence tests $\Delta t/\Delta x$ ratio was kept constant over a single test but was unique to each test.

Table 4: Test advection convergence subjected to tidal flow (Flux Limiter on)

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	CFL= 0.39
256	2.18E-5	6.21E-6	1.91E-3	2.39	2.47	1.49	Maximum Velocity = 0.43 m/s
128	1.15E-4	3.44E-5	5.38E-3				Flux Limiter: On
64	4.53E-4	1.77E-4	1.35E-2	2.36	2.36	1.32	BC Neumann Zero Flux

3-3. Diffusion

Diffusion governing equation is discretized in mass conservative form. Classic 2nd order implicit Crank-Nicolson finite volume, face center approach was adopted[xv]. The details are provided in addendum. Diffusion of Gaussian distribution of mass, and the test case by Fletcher (1991)[xvi] were tested with Dirichlet and Neumann boundary conditions.

Table 5: Diffusion of Gaussian hump of mass, subjected to Neumann BC

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	Mesh Peclet Number:
256	5.48E-6	4.09E-7	1.17E-5	2.00	2.50	1.99	7.90
128	2.19E-5	2.31E-6	4.69E-5				D= 0.1 m2/s
64	8.77E-5	1.31E-5	1.87E-4	2.00	2.50	1.99	BC Neumann analytical

[xv] Detail of discretization in Appendix A-2.
[xvi] Appendix B.

Table 6: Diffusion of Gaussian hump of mass, subjected to Dirichlet BC

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	Mesh Peclet Number:
256	1.14E-6	8.11E-8	2.08E-6	2.00	2.50	1.99	7.90
128	4.56E-6	4.58E-7	8.34E-6				D= 0.1 m2/s
64	1.82E-5	2.59E-6	3.33E-5	2.00	2.50	1.99	BC Dirichlet
							analytical

Table 7: Diffusion of smooth hump of mass, subjected to Neumann BC

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	Mesh Peclet Number:
256	1.11E-5	1.79E-6	5.29E-4	1.99	2.50	1.98	0.131
128	4.44E-5	1.01E-5	2.08E-3				D= 10.5 m2/s
64	1.75E-4	5.81E-5	7.80E-3	1.98	2.52	1.90	BC Neumann
							analytical

3-4. Reaction

The reaction ODE solver is the adoptive Heun 2-3 order explicit which is implemented inside the advection solver to attenuate mass balance error which had been mentioned in literature (Valocchi 1992). The explicit Runge-Kutta 3rd order and 2nd order *TGA* (Twizell et al. 1996) for dealing with stiff source terms are also coded[xvii].

[xvii] Detail of discretization in Appendix A-3.

Table 8: ODE reaction solver test, Heun 2nd order

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	
64	1.280E-5	6.404E-6	1.280E-5	2.01	2.50	2.01	First order decay
32	5.142E-5	3.636E-5	5.142E-5				
16	2.071E-4	2.071E-4	2.071E-4	2.00	2.52	2.00	

Table 9: ODE reaction solver test, RK 3rd order

Number of nodes	Error			Convergence $\log_3(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	
64	5.833E-7	2.916E-7	5.833E-7	3.02	3.02	3.02	First order decay
32	4.727E-6	2.363E-6	4.727E-6				
16	3.879E-5	1.939E-5	3.879E-5	3.61	3.61	3.61	

Table 10: Coupling ODE reaction solver, 2nd order and advection of mass

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	Linear decay Max Velocity 1.6 m/s CFL= 0.3
64	1.91E-6	1.64E-7	2.60E-5	1.97	2.47	1.97	
32	7.47E-6	9.11E-7	1.02E-4				
16	2.91E-5	5.05E-6	4.04E-4	1.98	2.47	1.96	

3-5. Advection-Diffusion-Reaction

Three operators are coupled directly (Godunov Splitting), for advection with uniform flow, linear decay and diffusion of a Gaussian hump of mass. Which are subjected to trivial constant flux (zero order approximation at far boundary).

Table 11: Coupling Advection Diffusion and Reaction Solvers (Flux Limiter off)

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	Linear decay CFL = 0.81 Max Velocity = 2.9 m/s Grid Peclet Num: 0.79 Peclet # =85
1800	2.417E-6	2.362E-7	7.28E-5	1.91	2.41	1.90	
900	9.099E-6	1.257E-6	2.73E-4				
450	3.179E-5	6.213E-6	9.46E-4	1.80	2.30	1.79	

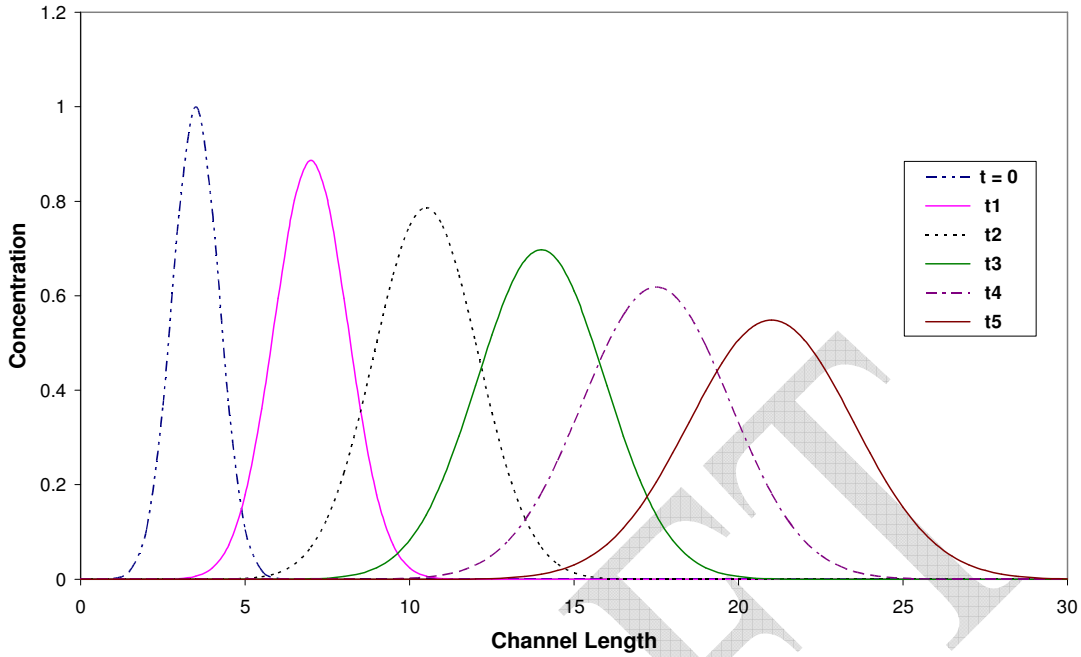

Figure 11: Coupling Advection, Diffusion and Reaction with trivial zero flux boundary condition

3-6. Advection-Diffusion-with Zero Order Boundary Condition

In the next step the different intermediate boundary condition approximation will feed to model and the accuracy and convergence ratio will assessed based on the dimensionless numbers and the intermediate step BC approximations figure 7.

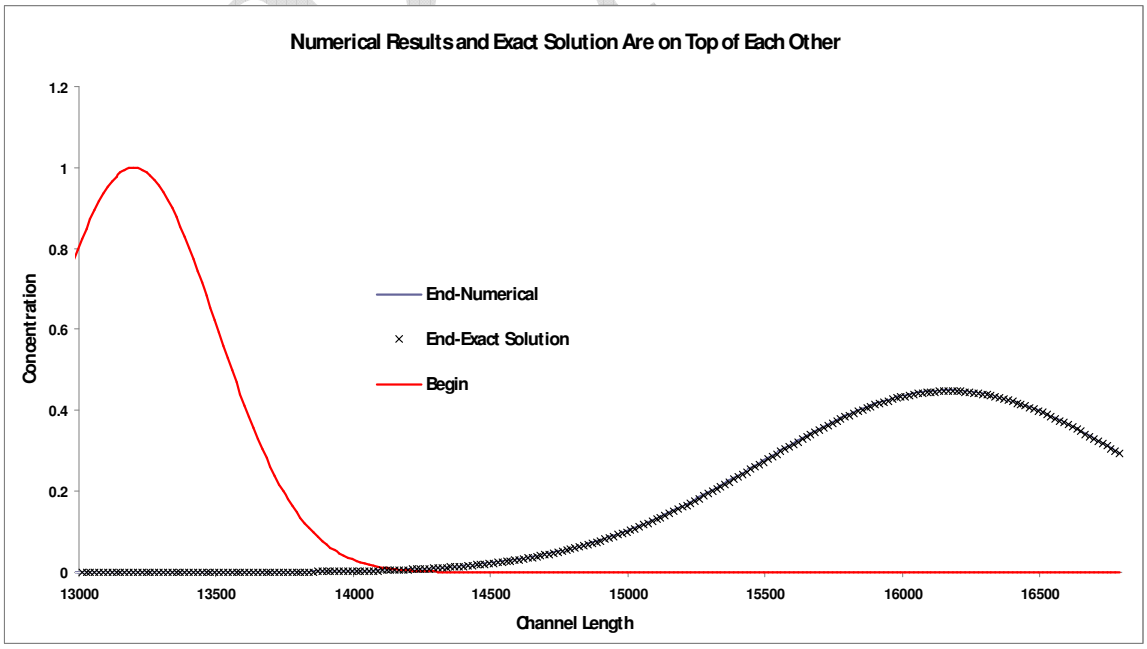

Figure 12: Coupling advection and diffusion with zero order implementation of intermediate boundary condition, L_1 error norm convergence ratio drops from *1.91* to *1.02*.

Table 11 shows the result for zero order approximation of intermediate BC for coupling the Advection and Diffusion.

Table 12: Coupling Advection and Diffusion Solvers with first Order approximation of the Intermediate Boundary Condition

Number of nodes	Error			Convergence $\log_2(L_{fine}/L_{Coarse})$			Note
	L_1	L_2	L_∞	L_1	L_2	L_∞	
512	1.19E-03	1.12E-04	9.65E-03	1.02147973	1.52105	1.02148	CFL = 0.75 Max Velocity = 2.9 m/s Flux Limiter: Off Grid Peclet Num: 0.79 Peclet Number[xviii] =120
256	2.46E-03	3.29E-04	1.77E-02				
128	5.38E-03	1.05E-03	3.93E-02	1.04264434	1.54102	1.03562	

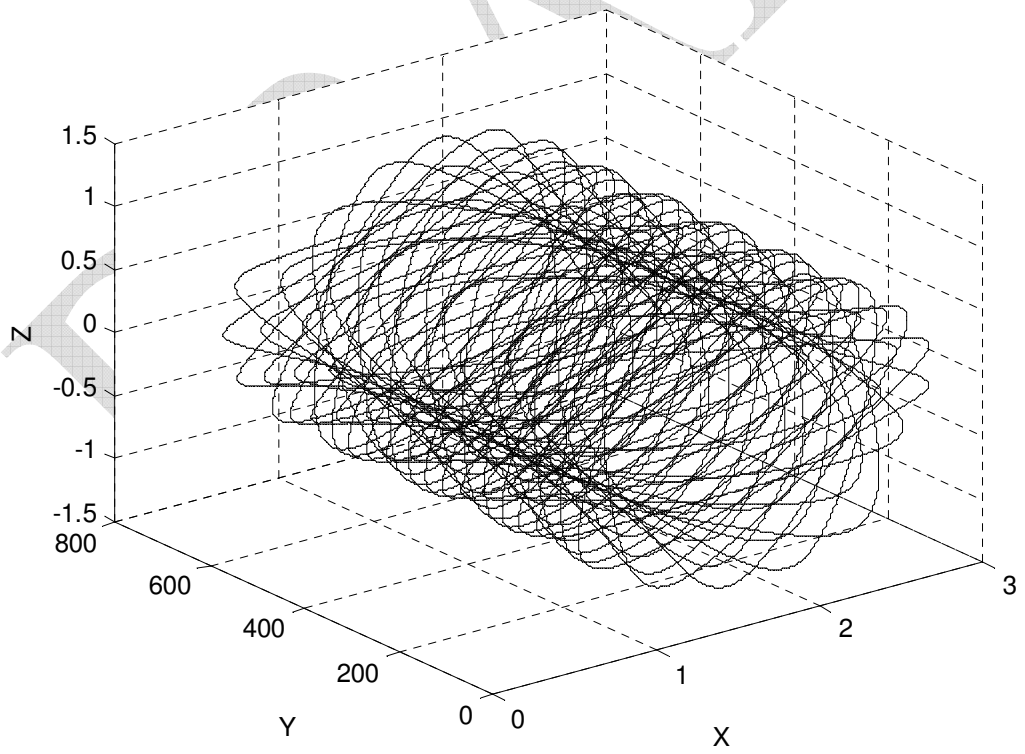

Figure 13: System of ODEs solved by the RK3 subroutine; finding the attractors (Zamani, 2010)

[xviii] Here the characteristic length was chosen as the domain length.

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Appendix A-1: Advection, Lax Two Steps Method

$$\frac{\partial(AC_s)}{\partial t}+\frac{\partial(QC_s)}{\partial x}=\frac{\partial}{\partial x}\left(AK_s\frac{\partial(C_s)}{\partial x}\right)+S/S=D+S/S \tag{A1.1}$$

A,Q,S, and K_s are known from other parts:
A and Q from HYDRO
K_s from Diffusion
S (Sink and source come from decay, deposition and entrainment)
1- First half step:

$$\overline{C}_{i\pm1/2}^{n+1/2}=C_i^n+\frac{\partial C_i^n}{\partial x}\frac{\Delta x}{2}+\frac{\partial C_i^n}{\partial t}\frac{\Delta t}{2}=C_i^n+\frac{1}{2}\left(\pm1-\frac{\Delta t}{\Delta x}\frac{Q}{A}\right)\Delta C_i^n \tag{A1.2}$$

Where

$$\Delta C_i^n=\frac{\partial C}{\partial x}\Delta x=D(C_{\lim ited})_i^n\times dx$$

$$D(C_{\lim ited})_i^n=function\quad of\quad (C_{i+1}^n,C_i^n,C_{i-1}^n)$$

$$r_i=\frac{C_i-C_{i-1}}{C_{i+1}-C_i}$$

$$\begin{cases} D(C_{\lim ited})_i^n=\dfrac{C_i-C_{i-1}}{\Delta x}-\phi\times\left[\dfrac{C_i-C_{i-1}}{\Delta x}-\dfrac{C_{i+1}-C_{i-1}}{2\Delta x}\right] \\ \phi=\left[\dfrac{r+|r|}{1+|r|}\right] \end{cases} \qquad (van\ Leer\ flux\lim iter)$$

$$C_{i\pm1/2}^{n+1/2}=\overline{C}_{i\pm1/2}^{n+1/2}+\frac{\Delta t}{2A}(S_i^n+D_i^n)$$

$$where\ D_i^n=\frac{AK_s\left.\dfrac{\partial C}{\partial x}\right|_{i+1/2}^{n}-AK_s\left.\dfrac{\partial C}{\partial x}\right|_{i-1/2}^{n}}{\Delta x}$$

$$D_i^n=\frac{(AK_s)_{i+1/2}^n\left\{(C_s)_{i+1}^n-(C_s)_i^n\right\}-(AK_s)_{i-1/2}^n\left\{(C_s)_i^n-(C_s)_{i-1}^n\right\}}{\Delta x^2} \tag{A1.3}$$

2- Second half step:

$$\overline{AC}_i^{n+1}=AC_i^n-\Delta t\times\frac{QC_{i+1/2}^{n+1/2}-QC_{i-1/2}^{n+1/2}}{\Delta x}+\Delta t\times S(C_i^n)$$

$$AC_i^{n+1}=AC_i^n-\Delta t\times\frac{QC_{i+1/2}^{n+1/2}-QC_{i-1/2}^{n+1/2}}{\Delta x}+\frac{\Delta t}{2}\times\left[S(C_i^n)+S(\overline{C}_i^{n+1})\right] \tag{A1.4-a,b}$$

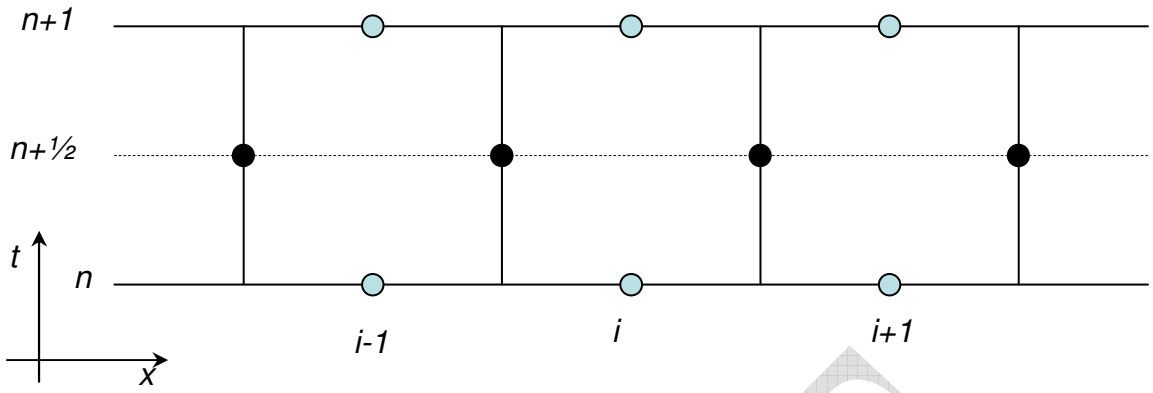

Figure A1: schematic of lax two step method

Flux limiter:

Flux limiters (slope limiters) are used in high resolution schemes, to avoid the spurious oscillations (wiggles) that would otherwise occur with high order spatial discretization schemes due to shocks, discontinuities or sharp changes in the solution domain.

van Leer (1977) flux limiter is one of the widely used limiters, which guarantees no new maximum/ minimum formed, and it could be formulated as follows for coding proposes: (Saltzman 1994).

1- Second order van Leer flux limiter:

$$\bar{\Delta}_i u = \begin{cases} \delta \,\mathrm{sgn}(u_{i+1} - u_{i-1}) & if\ \ \Delta_R u_i \times \Delta_L u_i > 0 \\ 0 & ,otherwise \end{cases} \qquad \text{(A1.5)}$$

Where:

$\delta = \min(2|\Delta_R u_i|, 2|\Delta_L u_i|, \frac{1}{2}|\Delta_C u_i|)$

$\Delta_R u_i = u_{i+1} - u_i$

$\Delta_L u_i = u_i - u_{i-1}$

$\Delta_C u_i = u_{i+1} - u_{i-1}$

And the limited flux will be:

$\Delta_i \bar{u} / dx$

2- Fourth order van Leer flux limiter:

$$\bar{\Delta}_i u = \begin{cases} \delta \,\mathrm{sgn}(u_{i+1} - u_{i-1}) & if\ \ \Delta_R u_i \times \Delta_L u_i > 0 \\ 0 & ,otherwise \end{cases} \qquad \text{(A1.6)}$$

where:

$\delta = \min\left\{2|\Delta_R u_i|, 2|\Delta_L u_i|, \frac{2}{3}|\Delta_C u_i| - \frac{1}{4}(\bar{\Delta}_i u_{i+1} + \bar{\Delta}_i u_{i-1})\right\}$

Note: $\overline{\Delta}_i u_{i+1}$ and $\overline{\Delta}_i u_{i-1}$ are the u which are already 2^{nd} order flux limiter applied on them

And the limited flux will be: $\Delta_i \overline{u} / dx$

Appendix A-2: Diffusion, Crank-Nicolson Method

$$\frac{\partial(AC_s)}{\partial t} = \frac{\partial}{\partial x}(AK_s \frac{\partial C_s}{\partial x}) \tag{A2.1}$$

$$\left\{ \frac{(AC_s)_i^{n+1} - (AC_s)_i^n}{\Delta t} = \theta \left[\frac{(AK_s)_{i+1/2}^{n+1} (\frac{\partial C_s}{\partial x})_{i+1/2}^{n+1} - (AK_s)_{i-1/2}^{n+1} (\frac{\partial C_s}{\partial x})_{i-1/2}^{n+1}}{\Delta x} \right] + \right. \tag{A2.2}$$

$$\left. (1-\theta) \left[\frac{(AK_s)_{i+1/2}^{n} (\frac{\partial C_s}{\partial x})_{i+1/2}^{n} - (AK_s)_{i-1/2}^{n} (\frac{\partial C_s}{\partial x})_{i-1/2}^{n}}{\Delta x} \right] \right.$$

C_i^{n+1} is unknown in (A2.2) and other terms are known from measurements or previous step.

$$F_{i\pm 1/2}^t \equiv -AK_s \frac{\partial C_s}{\partial x}\Big|_{i\pm 1/2}^t \tag{A2.3}$$

In which F is diffusive flux re-writing (A3.2) yields:

$$(AC_s)_i^{n+1} = (AC_s)_i^n - \theta\Delta t \left[\frac{F_{i+1/2}^{n+1} - F_{i-1/2}^{n+1}}{\Delta x} \right] - (1-\theta)\Delta t \left[\frac{F_{i+1/2}^{n} - F_{i-1/2}^{n}}{\Delta x} \right] \tag{A2.4}$$

1- Neumann Boundary condition implementation

$$F_{boundary} = -AK_s\Big|_{hydro} \frac{\partial C_s}{\partial x}\Big|_{known}$$

Just by replacing F in the first and last diffusive flux Neumann Boundary condition will be implemented

- Middle row will be:

$$\left(\frac{-\theta\Delta t}{\Delta x^2}(AK_s)_{i-1/2}^{n+1} \quad A_i^{n+1} + \frac{\theta\Delta t}{\Delta x^2}(AK_s)_{i+1/2}^{n+1} + \frac{\theta\Delta t}{\Delta x^2}(AK_s)_{i-1/2}^{n+1} \quad \frac{-\theta\Delta t}{\Delta x^2}(AK_s)_{i+1/2}^{n+1} \right)_{1\times 3} \times \begin{pmatrix} C_{i-1}^{n+1} \\ C_i^{n+1} \\ C_{i+1}^{n+1} \end{pmatrix}_{3\times 1} =$$

$$\left((AC_s)_i^n + \frac{(1-\theta)\Delta t}{\Delta x^2} \left\{ (AK_s)_{i+1/2}^n (C_s)_{i+1}^n - (AK_s)_{i+1/2}^n (C_s)_i^n - (AK_s)_{i-1/2}^n (C_s)_i^n + (AK_s)_{i-1/2}^n (C_s)_{i-1}^n \right\} \right)_{1\times 1} \tag{A2.5}$$

$$= \left((AC_s)_i^n - \frac{(1-\theta)\Delta t}{\Delta x}\left\{F_{i+1/2}^n - F_{i-1/2}^n\right\}\right)_{1\times 1} = (AC_s)_i^n - (1-\theta)\Delta t\{\text{explicit diffusive op}\} \quad (A2.5')$$

- First row: *i=1*

$$\left(A_1^{n+1} + \frac{\theta\Delta t}{\Delta x^2}(AK_s)_{3/2}^{n+1} \quad \frac{-\theta\Delta t}{\Delta x^2}(AK_s)_{3/2}^{n+1}\right)_{1\times 2} \times \begin{pmatrix} C_1^{n+1} \\ C_2^{n+1} \end{pmatrix}_{2\times 1} = \quad (A2.6)$$

$$\left(AC_1^n - \frac{(1-\theta)\Delta t}{\Delta x}\left(F_{3/2}^n - F_{1/2}^{n*}\right) + \frac{\theta\Delta t}{\Delta x}F_{1/2}^{n+1*}\right) (*: \textit{known b}\mathbf{o}\textit{undary})$$

- Last row*: i=m*

$$\left(\frac{-\theta\Delta t}{\Delta x^2}(AK_s)_{m-1/2}^{n+1} \quad A_m^{n+1} + \frac{\theta\Delta t}{\Delta x^2}(AK_s)_{m-1/2}^{n+1}\right)_{1\times 2} \times \begin{pmatrix} C_{m-1}^{n+1} \\ C_m^{n+1} \end{pmatrix}_{2\times 1} = \quad (A2.7)$$

$$\left(AC_m^n - \frac{(1-\theta)\Delta t}{\Delta x}\left(F_{m+1/2}^{n*} - F_{m-1/2}^n\right) - \frac{\theta\Delta t}{\Delta x}F_{m+1/2}^{n+1*}\right)$$

2- Dirichlet Boundary condition implementation

We assume the C is known on the face of first/last cells (edges of channel)

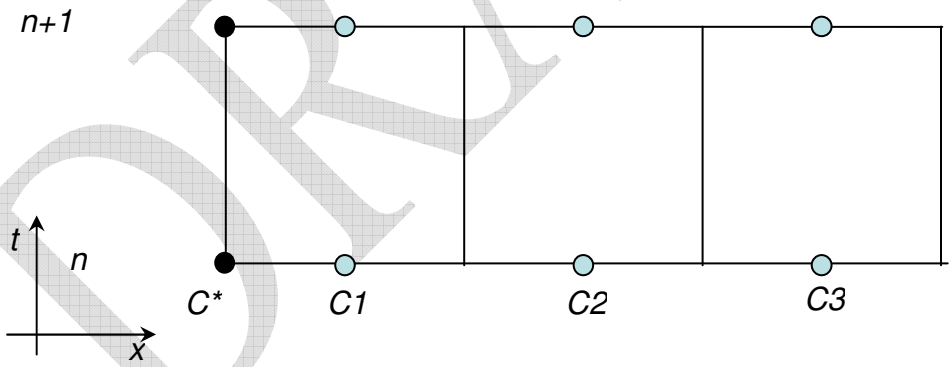

Figure A2: Schematic of boundary condition implementation

2.1- c(x) = a + bx+dx^2 (quadratic)

what we need is $\left.\frac{\partial C(x)}{\partial x}\right|_{x=0} = b + 2d(0) = b$ (A2.8)

1-at x=0 → c(0) = a+ b(0)+d(0) =a=c*

2-at x=Δx /2 → c(1/2) = c* +bΔx /2+ dΔx /4

3-at x=3Δx /2 → c(3/2) = c*+3bΔx /2+ 9dΔx /4

where b, d, c(1/2) and c(3/2) are unknowns.

If we eliminate d between equations 2, and 3 above, regardless of time.

$$b = \frac{9c_{x=1/2} - c_{x=3/2} - 8c^*}{3\Delta x} = \frac{9c_1 - c_2 - 8c^*}{3\Delta x} \tag{A2.9}$$

The only known value in the above is c* = c at the boundary, by replacing in (A2.6-7) we may compute the changes in coefficient and right hand side matrices.

2.2- c(x) = a + bx (linear)

what we need is $\left.\frac{\partial C(x)}{\partial x}\right|_{x=0} = b$ (A2.10)

1- at x=0 → c(0) = a + b(0) = c*

2- at x=Δx/2 → c(1/2) = a +bΔx /2 =c* + bΔx /2

→ b = (2c(1/2) – 2c*)/ Δx

where b and c(1/2) are unknowns and C* is the known value of the boundary

- **Dirichlet Boundary Condition**

For the left boundary,

$$\frac{\partial C}{\partial x} = b = \frac{2C(1) - 2C^*}{\Delta x} \Rightarrow F_{1/2} = -2AK_{1/2}\frac{C_1 - C^*_{boundary}}{\Delta x} \tag{A2.11}$$

The right boundary, $\frac{\partial C}{\partial x} = b = \frac{2C^* - 2C(n)}{\Delta x} \Rightarrow F_{m+1/2} = -2AK_{m+1/2}\frac{C^*_{boundsry} - C_m}{\Delta x}$ (A2.12)

- Middle row: is the same as previous case
- First row : *i=1*

$$\left(A_1^{n+1} + \frac{\theta\Delta t}{\Delta x^2}(AK_s)^{n+1}_{3/2} + \frac{2\theta\Delta t}{\Delta x^2}(AK_s)^{n+1}_{1/2} \qquad \frac{-\theta\Delta t}{\Delta x^2}(AK_s)^{n+1}_{3/2}\right)_{1\times 2} \times \begin{pmatrix} C_1^{n+1} \\ \\ C_2^{n+1} \end{pmatrix}_{2\times 1} =$$

$$\left(AC_1^n - \frac{(1-\theta)\Delta t}{\Delta x}\left(F^n_{3/2} - F^{n^*}_{1/2}\right) + \frac{2\theta\Delta t}{\Delta x^2}AK^{n+1}_{1/2}C^{*^{n+1}}\right)$$

(A2.13)

- Last row: *i=m*

$$\begin{pmatrix} \dfrac{-\theta\Delta t}{\Delta x^2}(AK_s)^{n+1}_{m-1/2} & A^{n+1}_m + \dfrac{\theta\Delta t}{\Delta x^2}(AK_s)^{n+1}_{m+1/2} + \dfrac{2\theta\Delta t}{\Delta x^2}(AK_s)^{n+1}_{m-1/2} \end{pmatrix}_{1\times 2} \times \begin{pmatrix} C^{n+1}_{m-1} \\ \\ C^{n+1}_m \end{pmatrix}_{2\times 1} = \qquad \text{(A2.14)}$$

$$\left(AC^n_m - \frac{(1-\theta)\Delta t}{\Delta x}\left(F^{n^*}_{m+1/2} - F^n_{m-1/2} \right) + \frac{2\theta\Delta t}{\Delta x^2} AK^{n+1}_{m+1/2} C^{*n+1} \right)$$

Appendix A-3: ODE Integrators

- **2nd order Heun method**:

$$C_i^{n+1} = C_i^n + \frac{1}{4(K_1 + 3K_2)} \qquad \text{(A3.1)}$$
$$\begin{cases} K_1 = \Delta t f(i,n) \\ K_2 = \Delta t f\left(i + {}^{2K1}/_{3}, n + {}^{2}/_{3}\right) \end{cases}$$

- **Runge-Kutta adoptive 3rd Order:**

This method is a third order Runge-Kutta method for approximating the solution of the initial value problem (Bogacki and Shampine, 1989).

$$\frac{dC}{dt} = f(x,t) \;\; subjected\ to\ C(x, t=0) = C_0$$

which evaluates the integrand, *f(x,y),* three times per step. For step *i+1*,
This method is a third order procedure for which Richardson extrapolation can be used.

$$C_i^{n+1} = C_i^n + \frac{1}{6(K_1 + 4K_2 + K_3)} \qquad \text{(A3.2)}$$
$$\begin{cases} K_1 = \Delta t f(i,n) \\ K_2 = \Delta t f\left(i + {}^{K_1}/_{2}, n + {}^{1}/_{2}\right) \\ K_3 = \Delta t f(i - K_1 + 2K_2, n+1) \end{cases}$$

- **Nystrom Method 3rd order**

$$C_i^{n+1} = C_i^n + \frac{1}{8(2K_1 + 3K_2 + 3K_3)} \qquad \text{(A3.3)}$$
$$\begin{cases} K_1 = \Delta t f(i,n) \\ K_2 = \Delta t f\left(i + {}^{2K_1}/_{3}, n + {}^{2}/_{3}\right) \\ K_3 = \Delta t f\left(i + {}^{2K_2}/_{3}, n + {}^{2}/_{3}\right) \end{cases}$$

- **Optimum method 3rd order**

$$C_i^{n+1} = C_i^n + \frac{1}{9(2K_1 + 3K_2 + 4K_3)} \qquad \text{(A3.4)}$$
$$\begin{cases} K_1 = \Delta t f(i,n) \\ K_2 = \Delta t f\left(i + {}^{K_1}/_{2}, n + {}^{1}/_{2}\right) \\ K_3 = \Delta t f\left(i + {}^{3K_2}/_{4}, n + {}^{3}/_{4}\right) \end{cases}$$

- **Heun 3rd order**

$$C_i^{n+1} = C_i^n + \frac{1}{4(K_1 + 3K_3)} \qquad \text{(A3.5)}$$
$$\begin{cases} K_1 = \Delta t f(i,n) \\ K_2 = \Delta t f\left(i + {}^{K_1}/_{3}, n + {}^{1}/_{3}\right) \\ K_3 = \Delta t f\left(i + {}^{2K_2}/_{3}, n + {}^{2}/_{3}\right) \end{cases}$$

Adaptive step size ODE integrator

A good ODE integrator should exerts some adaptive control over its own progress, making frequent changes in its step size. Usually the purpose of this adaptive step size control is to achieve some predetermined accuracy in the solution with minimum computational effort. The whole transport engine is coded double precision so our goal in solving the stiff source terms is we could achieve a precision equal to or higher than the other parts (in our case epsilon = 10^{-10}). The strategy to find the required length of sub-step-which ends up to a preset accuracy- is called *Richardson Extrapolation*.

The principle definition of "order of convergence" is based on behavior of the error of discrete solution. There are various measures (L_1, L_2, L_∞), but in some sense we are always referring to the difference between discrete solution f(Δ) and the exact solution:

$$E = f(\Delta) - f_{exact} \tag{A3.6}$$

For an order p method, and for a well-behaved problem, the error in the solution E asymptotically will be proportional to Δ^P. This terminology applies to every "consistent" methodology regardless of solution smoothness, thus

$$E = f(\Delta) - f_{exact} = C\Delta^P + H.O.T \tag{A3.7}$$

where H.O.T are higher order terms.

Example:

Let's assume we run the 2nd order Huen method with step size Δt = *0.2* and receive an approximation of *6.59862478489*, and then we run the same solver for the step size Δt = *0.1* and received an approximation of *6.59854357165*. The question is if we are seeking the solution with the accuracy of 10^{-8} what is the integration step size?

$$u_{exact} = 6.59854357165 + C(0.1)^2 + H.O.T$$
$$u_{exact} = 6.59862478489 + C(0.2)^2 + H.O.T$$

Subtracting the above we have:

$$0.00008121324 + C(0.2)^2 - C(0.1)^2 + H.O.T = 0$$

$$0.00008121324 + 0.03C \approx 0 \Rightarrow C = -0.002707108$$

So to achieve an error of 10^{-8} with Heun 2nd order integrator we need:

$$C(\Delta t)^2 + O(\Delta t)^3 = 10^{-8} \Rightarrow \Delta t \le \sqrt{\frac{10^{-8}}{0.00270718}} = 0.00192$$

Appendix B: Benchmark Analytical Solutions

1. The Advection Diffusion Reaction equation:

$$\frac{\partial C}{\partial t} + \frac{\partial (UC)}{\partial x} - \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) = -\lambda C \tag{B.1}$$

Has an analytical solution of:

$$C(x,t) = \frac{e^{-\lambda t - \frac{(x-ut)^2}{4Dt}}}{\sqrt{4\pi Dt}} \tag{B.2}$$

The initial and boundary condition could be derived from (B-2), (Sobey 1989; Khan and Liu 1995)

2. ADR solution by Zoppou and Knight 1997:

$$\frac{\partial C(x,t)}{\partial t} + \frac{\partial [C(x,t)u_0 x]}{\partial x} = \frac{\partial}{\partial x}\left(D_0 x^2 \frac{\partial C(x,t)}{\partial x}\right) \tag{B.3}$$

This is subjected to:

$$\begin{cases} x_0 < x \le \infty \ , t > 0, \\ c(x,0) = 0 \ \ for \ \ x > x_0 \ , \ c(x_0,t) = C_0 \quad for \ \ x \le x_0 \\ c(\infty,t) = 0 \end{cases}$$

The solution is

$$C(x,t) = \frac{C_0}{2}\left\{\frac{x_0}{x} erf\left[\frac{\ln(\frac{x_0}{x}) - t(u_0 + D_0)}{2\sqrt{D_0 t}}\right] + \exp\left[\frac{u_0 \ln(\frac{x_0}{x})}{D_0}\right] erf\left[\frac{\ln(\frac{x_0}{x}) + t(u_0 + D_0)}{2\sqrt{D_0 t}}\right]\right\} \tag{B.4}$$

3. ADR solution by Fletcher (1991):

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{B.5}$$

Has the analytical solution of:

$$c(x,t) = 2x + 4\cos\left(\frac{\pi}{2}x\right)\exp\left[-D\left(\frac{\pi}{2}\right)^2 t\right] \tag{B.6}$$

The initial and boundary condition could be derived based on (B.6).

4. Analytical solution of tidal forcing in a rectangular basin (Wang et al., 2009)

Governing equation in 2D (X-Z):

1-Continuity

$$u_x + w_z = 0$$

$$\zeta_t + u_x H = 0$$

Assumptions:

- u, is not function of z but vertical velocity w is a function of z
- H is constant
- Z << H

2- Momentum

$$u_x + g\zeta_x = 0$$

Assumptions:

- Inviscid fluid (interfacial and bottom friction are neglected)
- P=constant
- Non-rotating reference frame (f=0)
- $uu_x \ll u_t , g\zeta_t$
- *The analytical solution for the u is:*

$$\begin{cases} u(x,t) = \left[\left(a\frac{\sqrt{gH}}{H}\right) \Big/ \cos\left(\frac{\omega_t}{\sqrt{gH}}L\right)\right] \sin\left(\frac{\omega_t}{\sqrt{gH}}(L-x)\right)\sin(\omega_t t) \text{ , Rueda, F. J. and Smith, P. E. (2009)} \\ \frac{dx}{dt} = u(x,t) \end{cases}$$

$$\left[\left(a\frac{\sqrt{gH}}{H}\right) \Big/ \cos\left(\frac{\omega_t}{\sqrt{gH}}L\right)\right] = A \qquad \text{and} \qquad \frac{\omega_t}{\sqrt{gH}} = B$$

$$\frac{dx}{dt} = A\sin(B(L-x))\sin(\omega_t t)$$

Integration will result in:

$$\ln\left(2\cot\frac{B(L-x)}{2}\right) = \frac{-AB}{\omega_t}\cos(\omega_t t) + Const.$$

Subjected to the boundary condition $u(L,t)$=0

$$x(t) = L - \frac{2}{B}\,Arccot\left\{\frac{1}{2}K_0\, e^{\frac{-BA}{\omega_t}\cos(\omega_t t)}\right\}$$

K_0 must be calculated base on boundary conditions

@t=0 : $$x_0 = x(t=0) = L - \frac{2}{B}\, Arccot\left\{\frac{1}{2}K_0\, e^{\frac{-BA}{\omega_t}}\right\}$$

$$K_0 = 2e^{\frac{BA}{\omega_t}}\, cot\left\{\frac{B(x_0 - L)}{2}\right\}$$

Appendix C-1: Sediment Entrainment and Deposition Functions

Under appropriate simplifying assumptions, the one dimensional St. Venant shallow water equation takes the form:

$$\frac{\partial A}{\partial t}+\frac{\partial UA}{\partial x}=q_{lateral} \tag{C1.1a}$$

$$\frac{\partial UA}{\partial t}+\frac{\partial U^2A}{\partial x}=-gA\frac{\partial h}{\partial x}+gAS-C_fU^2B \tag{C1.1b}$$

Where; t: time; x: boundary-attached (bed attached) streamwise coordinate; g: gravitational acceleration; S: bed slope which is given; $S=-\frac{\partial \eta}{\partial x}$;C_f: bed friction coefficient. The river assumed to carry a dilute suspension of sediment. An approximate form of depth averaged conservation of suspended sediment is as follows:

$$\frac{\partial CA}{\partial t}+\frac{\partial UCA}{\partial x}=\frac{\partial}{\partial x}\left(\frac{ACK_s}{\partial x}\right)+E_r-D_r=\frac{\partial}{\partial x}\left(\frac{ACK_s}{\partial x}\right)+v_s(E_s-\bar{c}_b)B \tag{C1.2}$$

Where; v_s: is the sediment fall velocity, E_r: sediment entrainment rate, E_s: dimensionless rate of entrainment of bed sediment into suspension, $E_s \equiv E_r / v_s$, D_r: volume rate of deposition per unit time per unit width, $\bar{c}_b$ = near bed value of $\bar{c} = r_0 C$

In the steady, uniform turbulent flow over a flat bed the net vertical flux (F_{sz}) of sediment just above the bed is given by:

$$\bar{F}_{sz}\big|_{z=b}=E_r-D_r=v_s(E_s-\bar{c}_b) \tag{C1.3}$$

$\Rightarrow \quad \bar{F}_{sz}<0$: *no deposition*

$\Rightarrow \quad \bar{F}_{sz}>0$: *no erosion*

If equilibrium steady uniform suspension rate exists, there is no net normal flux of suspended sediment at the bed. The equilibrium condition yields $\bar{F}_{sz}=0$, $E_s = \bar{c}_b$ hence the entrainment rate will be given by $\bar{c}_b$.

There are many formulas for concentration sources near bed, the following formulas were widely recommended in the literature:

Entrainment Formulas

1. Garcia and Parker

In 1991, Garcia and Parker suggest the following formula:

$$E_s = \frac{AZ_u^5}{1+\frac{A}{0.3}Z_u^5} \tag{C1.4}$$

E_s= Sediment entrainment coefficient

$$A = 1.3\times10^{-7} \tag{C1.4.1}$$

$$Z_u = \frac{u_*}{\nu_s}\mathrm{Re}_p^{0.6} \tag{C1.4.2}$$

Z_u is a measure of the shear stress strength but it also takes into account the particle size. Here reference level is taken to be 5% of the depth.

$$u_* = \frac{g^{0.5}}{C'}U_m \tag{C1.4.3}$$

u_* : shear velocity

$$C' = 18\log\left(\frac{12R_b}{3D_s}\right) \qquad \textit{Chezy Coefficient} \tag{C1.4.4}$$

U_m= is the cross sectional flow velocity

R_b= Hydraulic radius of channel

v_s= sediment fall velocity (will discuss later in this appendix)

$$\mathrm{Re}_p = \frac{\sqrt{RgD}\,D}{\nu} \qquad \textit{and} \quad \mathrm{Re}_p < 3.5 \tag{C1.4.5}$$

Re_p is particle Reynolds number

$$R = \frac{\rho_s - \rho}{\rho} \tag{C1.4.6}$$

R is specific submerged gravity (*1.65* for quartz particle), g = Gravitational acceleration, $D = D_{50}$.

In Garcia and Parker (1991) a comparison of many of other entrainment formula could be found. They have found that the relation (C1.4) works well for fine-grained non-cohesive sediments.

2. van Rijn

Another formula that has been found to perform well is that of van Rijn (1984b).

$$\bar{c}_b = 0.015 \frac{D_s}{b} \frac{(\tau_s^* / \tau_c^* - 1)^{1.5}}{d_*^{0.3}} \tag{C.5}$$

$$d_* = D_s \left(\frac{gR}{\nu^2} \right)^{1/3} \tag{C.5.1}$$

$$b = \begin{cases} \Delta_b / 2 \; if \quad \Delta_b \; is \; known \\ k_s \; if \; \Delta_b \; is \; unknown \end{cases} \tag{C.5.2}$$

$$b_{\min} = 0.01H$$

$k_s=3D$ for uniform material (is effective roughness height), Δ is a bed forms height and $b=k_s$ when bed forms height is unknown, H: Total depth of flow, d_*= is dimensionless particle parameter , $\bar{c}_b$: Reference concentration for equilibrium case (near bed value of mean volumetric sediment concentration), $R = \frac{\rho_s - \rho}{\rho}$, D_s= D_{50}, g = Gravitational acceleration, Note: here τ_c^* denotes the dimensionless Shields stress due to skin friction (mobility parameter)

$$\tau_s^* = \frac{\tau_{bs}}{\rho R g D} \tag{C1.5.3}$$

$$\tau_{bs} = \rho C_{fs} U^2 \tag{C.15.4}$$

τ_{bs} is the shear stress caused by skin friction

$$C_{fs} = \frac{1}{\kappa} \ln \left(12 \frac{H}{k_s} \right)^{-2} \tag{C1.5.5}$$

In which, C_{fs} is the resistant coefficient, k_s is the effective roughness height, κ = von Karman constant (0.41), this formula has been used extensively in numerical treatment of suspended sediment transport (Duan et al., 2001; Zeng et al., 2006).

3. Smith and McLean

Third equation which performs well is by Smith and McLean (1977). This equation is based on Yalin early works (1963).

$$\bar{c}_b = 0.65\frac{\gamma_0(\tau_s^*/\tau_c^* - 1)}{1+\gamma_0(\tau_s^*/\tau_c^* - 1)} \quad \text{(C1.6)}$$

Where, $\bar{c}_b$: Reference concentration for equilibrium case, $\gamma_0 = 0.0024$, and the value of *b* (height in which the $\bar{c}_b$ is to be evaluated) is given by the following:

$$b = 26.3(\tau_s^*/\tau_c^* - 1)D + k_s \quad \text{(C1.6.1)}$$

k_s= is the equivalent roughness height for fixed bed

$$\tau_s^* = \frac{\tau_{bs}}{\rho RgD} \quad \text{(C1.6.2)}$$

τ_s^* is the dimensionless stress due to skin friction

$$\tau_{bs} = \rho C_{fs} U^2 \quad \text{(C1.6.3)}$$

τ_{bs} is the shear stress caused by skin friction

$$C_{fs} = \frac{1}{\kappa = 0.41}\ln\left(11\frac{H_s}{k_s}\right)^{-2} \quad \text{(C1.6.4)}$$

Here H_s is the depth in absence of bed forms (H_s+H_f=H) and H_s it could be expressed as:

$$H_s = \frac{U^2}{gS}\left[\frac{1}{\kappa}\ln\left(12\frac{H}{k_s}\right)\right]^{-2} \quad \text{(C1.6.5)}$$

κ= von Karman constant (0.41), K_s is the effective roughness height, *S:* energy slope, τ_c^* is dimensionless critical Shields shear stress for incipient motion (Appendix C-2).

The Smith and McLean formula is used extensively in benthic boundary layer flows and oceanic sedimentation (McCave, 2004).

4. Zyserman and Fredsoe

After the comparative analysis of different entrainment formulations, in 1994 Zyserman and Fredsoe proposed an empirical relation (C1.7) using the Fort Collins experimental data.

$$\bar{c}_b = \frac{0.331(\tau_s^*/\tau_c^* - 1)^{1.75}}{1+0.72(\tau_s^*/\tau_c^* - 1)^{1.75}} \quad \text{(C1.7)}$$

$\bar{c}_b$ here is referred to concentration at $b=2D_{50}$,

$\tau_s^* = \frac{\tau_{bs}}{\rho RgD}$, τ_s^* is the shields stress due to skin friction

$$\tau_{bs} = \rho C_{fs} U^2 \tag{C1.7.1}$$

$$C_{fs} = \frac{1}{\kappa} \ln\left(11 \frac{H_s}{k_s}\right)^{-2} \tag{C1.7.2}$$

Here H_s is the depth in absence of bed forms, (H_s+H_f=H) and H_s could be expressed as:

$$H_s = \frac{U^2}{gS}\left[\frac{1}{\kappa} \ln\left(12 \frac{H}{k_s}\right)\right]^{-2} \tag{C1.7.3}$$

κ = von Karman constant (0.41), S=energy slope, k_s is the effective roughness height, τ_c^* is dimensionless critical Shields shear stress for incipient motion.

This formula is based on laboratory data, but it has been used widely in costal engineering practice (Soulsby, 1997).

Appendix C-2: Fitted Formula to the Shields Diagram

C2-1: Brownlie (1981)

$$\tau_c^{*} = 0.22R_{ep}^{-0.6} + 0.06\exp\left(-17.77R_{ep}^{-.06}\right) \quad \text{(C2.1)}$$

Where; Re_p is particle Reynolds number, $R_{ep} = \frac{\sqrt{gRD}\ D}{\nu}$, $R = \frac{\rho_s - \rho}{\rho}$, $D = D_{50}$, g: gravitational acceleration, ν: kinematic viscosity of water, τ_c^{*} is dimensionless critical Shields shear stress for incipient motion.

C2-2: Mantz (1977)

For fine-grained sediments Shields diagram does not provide realistic results. Mantz conducted a series of experiments and observed that for fine grained non-cohesive sediments the critical shear stresses can be estimated with the following relation

$$\tau_c^{*} = 0.135R_{ep}^{-0.261} \qquad 0.056 < R_{ep} < 3.16 \quad \text{(C2.2)}$$

The Mantz equation merges Brownlie equation for $R_{ep}=4.22$

Appendix C-3: Fall Velocity

Fall velocity or settling velocity is a fundamental property of a sediment particle. Falling under the gravity action a particle will reach a constant, terminal velocity once the drag is equal to the submerged weight of the particle. The range of particle sizes can be categorized in three following sizes:

a) Medium and coarse sand, gravel, cobble, and boulder; $d_s>0.1$ *mm* which must be calculated with Rubey's approximation of fall velocity (Stokes' law is not valid for them)

b) Very fine Sand and Silt; $0.1\ mm > d_s > 0.004\ mm$ which can calculate by Stokes' law.

c) Clay; which is also calculated by Stokes' law but flocculation is possible.

Stokes' law:

It is valid for small particle size ($d_s<0.1$ *mm*) falling in viscous fluid ($Re_p<0.1$)

$$v_s = \frac{1}{18}\frac{(G-1)g}{\nu}d_s^2 \qquad R_{ep} < 0.1 \qquad \text{(C3.1)}$$

G is specific gravity and, $G = \frac{\rho_s}{\rho} = 2.65$ for quartz particle.

Rubey's Formula:

Rubey's approximation formula (C3.2) of fall velocity in clear water is based on drag coefficient of sand particle equation (C3. 3):

$$v_s = \frac{8\nu_m}{d_s}\left[(1+0.0139d_*^3)^{0.5}-1\right] \qquad \text{(C3.2)}$$

$$C_D = (24\nu_m / v_s d_s) + 1.5 \qquad \text{(C3.3)}$$

$$v_s = \frac{8\nu_m}{d_s}\left[(1+0.0139d_*^3)^{0.5}-1\right] \qquad \text{(C3.4)}$$

$$d_* = d_s\left[\frac{(G-1)g}{\nu_m^{\,2}}\right]^{1/3} \qquad \text{(C3.5)}$$

ν_m is the kinematic viscosity of water-sediment mixture, d_* is the dimensionless particle diameter, both Rubey's and Stokes' formula yield practically same results for the cases of Reynolds numbers less than one, so all the settling velocities will be calculated base on Rubey's approximation

Appendix C-4: Cohesive Sediment

Introduction:

Fine grained sediment transport is generally characterized by size composition, and plasticity. Cohesion is due to electrochemical forces acting on the particle surface. Hence the degree of cohesion depends on the ratio of particle surface area to particle weight, that is, specific surface area. Migniot (1968) showed ratio of particle settling velocity to particle size increases due to floc and cohesion.

A characteristic gauge of clay mineral cohesion is cation exchange capacity (CEC). The higher the CEC the greater the cohesion, which causes micro-meter-sized individual clay particles to coagulate or flocculate, in water to form much larger aggregates, or flocs when water salinity exceeds a critical value which depends on the clay mineral.

Kaolinite, illite, chlorite, and montmorillonite are the most commonly found clays, in the San Francisco Bay estuary Chlorite were found (Krone, 1962). As salinity increases above the critical value, floc size density, and strength vary. However, above a salinity of about 10 ppt, its effect on the floc properties is comparatively minor (Krone, 1962; 1986) and there is no need to take it into calculation.

Table C1: Clay Minerals. CEC, and Critical Salinity for Flocculation

Clay mineral	Nominal Diameter (μm)	CEC (meq/100 g)	Critical Salinity (ppt)
Kaolinite	0.36	3-15	0.6
Illite	0.062	10-40	1.1
Chlorite	0.062	24-35	Not reported
Montmorillonite	0.011	80-150	2.4

To make assessing of transport related data possible, the basic parameters of floc in cohesive sediment should be defined. Regarding the fact that the cost of evaluation of a large number of parameters is not feasible in most technical studies, finally six parameters have been chosen to be representative of characterization of sediment in the situation in which the transport is not overwhelmingly influenced by biochemical factors;

- Particle size: use the standard procedure of (ASTM 1993d), settling column bottom withdrawal test. If the organic content is greater than 10%, this test shouldn't perform
- Fall or settling velocity.
- Mineral decomposition: obtain types of relative quantities of the principle clay and non-clay minerals using standard X-ray diffraction tests.
- Organic content: Loss of sample mass on ignition standard test (ASTM 1993d) An alternative is to measure total organic carbon.
- Cation exchange capacity: follows standard procedure for clay minerals (ASTM 1993c, SCS 1992)
- Salinity: report salinity if less than about *10 ppt*, At higher salinity the effect of salinity on floc structure is comparatively minor.

Settling velocity of cohesive sediment

For hindered settling of mud flocs, Mehta (1986) suggested a modified for of the well known Richardson and Zaki formula:

$$v_s = v_{s,0}(1 - k\phi_p)^n \qquad \text{(C4.1)}$$

where v_s is the effective settling velocity, $v_{s,0}$ the settling velocity of a single particle in still water, k is an empirical parameter, φ_p is volumetric concentration of primary particle, $\varphi_p = C/\rho_s$ in which C is the mass concentration and ρ_s the density of the sediment.

Winterwerp (2002) reasoned that the rational embedded in (C4.1) can be applied to cohesive sediments as well. He suggested that, as each individual floc within a suspension is considered to settle in the rest of the suspension, this would result in three hindering effects:

1- Return flow and wake formation. A settling particle generates a return flow and a wake. Other neighboring particles will be influenced by this and their effective settling velocity will be decreased by a factor (1- φ), where φ is the volumetric concentration of flocs.

2- Viscosity. Each individual particle within a suspension is considered to fall in the remainder of that suspension which has an increased viscosity.

3- Buoyancy or reduced gravity. For the same argument, an individual particle settles in a suspension with an increased bulk density. The effective settling velocity is decreased by a factor of $(1-\varphi_p)$.

This led to a new theoretically derived formula for the hindered settling of mud flocs:

$$v_s = v_{s,0} \frac{(1-\phi)^m (1-\phi_p)}{1+2.5\phi} \qquad \text{(C4.2)}$$

where v_s is the effective settling velocity, $v_{s,0}$ the settling velocity of a single particle in still water. The volumetric concentration is herein related to the gelling concentration ($\phi \equiv C/C_{gel}$), in which C_{gel} is the concentration at which flocs become space-filling and form a network structure, called a gel, and a measurable strength build up. The volumetric concentration of primary particles is also related to the gelling concentration, $\phi_p = c/\rho_s = c_{gel}\varphi/\rho_s$

Here the $(1-\phi)$ accounts for the return-flow effect, $(1-\phi_p)$ accounts for the buoyancy effect and $(1+2.5\phi)$ accounts for augmented viscosity. The exponent "m" is an empirical parameter to account for possible non-linear effects. When the return flow effect is linear (m=1) only the volume effect of a suspension settling in a liquid is taken into account. The downward flux of sediment is thus expected to create an equal upward flux of water with sediment. When nonlinearity is taken into account, all the effects generated by a settling particle in a suspension are incorporated.

Winterwerp (2002) compared Eq (C4.2) to data by fitting the model parameter and not actually using parameter values derived from data. A reasonable fit was obtained.

Appendix D: Metrics for Determining Accuracy in CFD

When we are dealing with numbers we can identify them as being large or small. Arrays and vectors are functions of many elements but we need to measure their size -an index for them to be small or large. Norms are used as a measure in this context. Realizing that the size of a vector or matrix should depend on the magnitude of all elements in the arrays, we arrive at the definition of vector and matrix norms. By definition, a norm is a single number that depends on the magnitude of all elements in the vector or matrix. A norm for vectors should satisfy the following conditions:

1- $\|\vec{v}\| \geq 0$ *and* $\|\vec{v}\| = 0$ *if and only if* $\vec{v} = 0$. (D.1)

2- $\|c\vec{v}\| = |c|\|\vec{v}\|$ *for any scalar* c. (D.2)

3- $\|\vec{v} + \vec{w}\| \leq \|\vec{v}\| + \|\vec{w}\|$ *for vectors* $\vec{v}$ *and* $\vec{w}$. (D.3)

The equation (D.3) is the triangle inequality. The following three vector norms are commonly used and called the infinity, one and two vector norms:

1- $L_\infty = \|\vec{v}\|_\infty = \max|v_i|$ (D.4)

2- $L_1 = \dfrac{\sum_j \|\vec{v}\|_1}{n} = \dfrac{\sum_j^n \sum_i |v_i|}{n}$ (D.5)

3- $L_2 = \dfrac{\sum_j^n \left(\sum_i |v_i|^2 \right)^{1/2}}{n}$ (D.6)

In our case we can define **v** as the error between U_{exact} and $U_{\text{numerical}}$ at each point (Bathe, 1996).

If we can find constants $p \geq 1$ and $c > 1$ such that

$$\lim_{k \to \infty} \frac{|x_{k+1} - x|}{|x_k - x|^p} = c \quad \text{(D.7)}$$

we say that convergence is of order p. If $p=1$ convergence is linear and the rate of convergence is c, in which c must be smaller than 1. In solution procedures using vectors and matrices we also need a measure of convergence.

It can proven that $L_2 \leq L_1 \leq L_\infty$, or in the other words L_∞ is the most restrictive norm and the L_2 is the most forgiving norm among these three (Kollmann, 2009). L_2 is

sometimes also called energy norm and it denotes the scatter index between the benchmark and the other dataset. L_1 denotes the average error in the domain and L_∞ shows the worst case. It is generally impossible to obtain a simple closed form expression for the global error after hundreds or thousands of time steps. Instead of trying to obtain the error directly, the approach that is widely used in the study of numerical methods consists of a two-pronged attack on the problem:

- Study the error introduced in a single time step, showing that the method is *consistent* with the differential equation and introduces a small error in any one step.
- Show that the method is *stable*, so that these local errors do not grow catastrophically and hence abound on the global error can be obtained in terms of these local errors.

If we can get a bound on the error in an appropriate sense, then stability can be used to convert this into a bound on the global error that can be used to prove convergence. Moreover, we can generally determine the rate of convergence and perhaps even obtain reasonable error bounds. The *fundamental theorem* of *Godunov*[xix] type numerical methods for partial differential equations (*Lax Equivalence Theorem*) can then be summarized briefly as (Leveque, 2002):

$$Consistency + Stability \Leftrightarrow Convergence$$

So the *mesh refinement convergence study* must be done for the different processes to confirm both *consistency* and *stability* (Fletcher, 1991; Roache, 2009).

[xix] The Lax Theorem is rigorously proves for FDM, but it is valid for FVM. Also some people take it true for FEM (See Fletcher, 1991).