General Introduction

Many physical processes can´t be described by equations whose solutions are straightforward derived from analytical methods. In fact most real-world processes are only descriptible by or *modeled* through a complex set of partial differential equations with many variables which often are themselves coupled. Usually one would for instance investigate the time-space evolution of a process (i.e. the concentration profile of a flowing chemical solution) in a given physical setting (such as a radial symmetrical conduct) under a given set of initial conditions (i.e. a concentration value at a specific time and place under a given pressure gradient). From this simple, somehow contrived example, one realizes the complexity arising from portraying the process through a system of differential equations and then solving it. It is quite obvious, the solution to this problem isn´t straightforward derivable from analytical methods. To tackle this problem one should turn to *numerical methods* for an approximate mathematical solution. Fortunately an extensive literature body has been worked out on the theory of *numerical methods* over these past two hundred years, and thanks to today elaborated programming languages as well available computing horsepower, tremendous improvements have been made pertaining to the implementation of corresponding algorithms to achieve a fine-tuned error-margin of their set of solutions. Furthermore through various softwares one can even picture the computed set resulting from the differential system.

However portraying a process through a highly coupled partial differential equations system and then numerically solving it isn´t a trivial undertaking; it requires skills, which this Manual is about. Moreover the gained numerical solutions themselves aren´t worth if they fail to achieve consistency, that is if they fail to comply with physical requirements. Therefore thought should be given on deep understanding of the basic physical laws driving the process and particularly their logical implications, the validating criterion against the computed data. From this it becomes obvious that the causes of a non-consistent computed data are quite multiple: it may stem from an incorrect formulation or even misconception of the differential system, an inadequate or error-ridden numerical method, a mistake in the code design, a faulty code

procedure, a deficient programming or even an error in displaying the computed data.

Why engage in such error-prone task?

Modeling processes is in certain cases often the only way to get insights into the evolution of a given phenomenon because of the absence of any practical experience or experimental set-up to investigate it: we may call into mind weather forecasting, climate change and in other fields we may mention simulating the actions´ index fluctuations in a bourse.

Therefore mastering the subject is quite worth the effort.

Let us now for illustrative purposes consider again the said example of a flow to which an additive is sprayed in upon entering a given region of a tube and we are interested in knowing the additive´s concentration profile downwards: to simplify we assume the tube is of constant section, the flow *laminar*, i.e. non-turbulent, the velocity field being constant. We further take advantage of the radial symmetry, assuming the fluid being *isotropic* enables us to state that the concentration profile is radial-symmetrically distributed at any time, because the sole process superposing to the isotropic *diffusion* is *advection* due to the fluid velocity field itself. Moreover the flow velocity is minimal at the inner wall, due to friction and maximal at the center on the tube axis; because of the radial symmetry it will assume a parabolic shape and layered as we shall later demonstrate. This allows substituting the flow description in the tube with a simpler flow description in a 2D geometry as shown in Figure1.

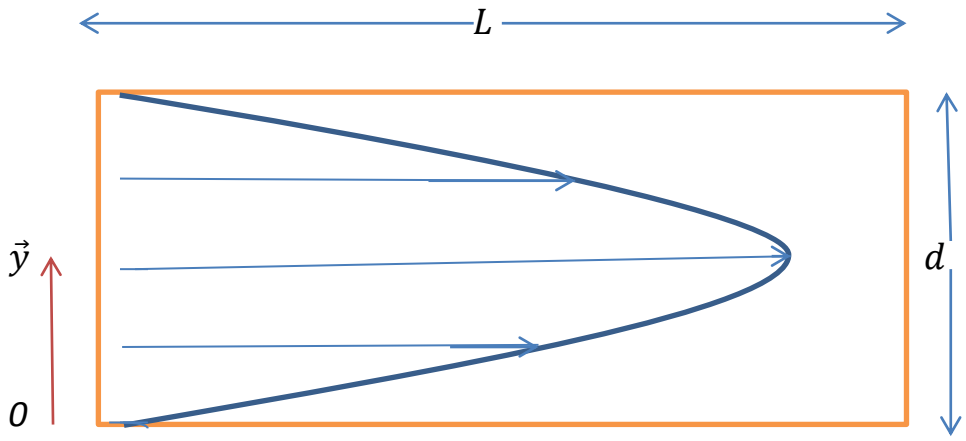

Figure1: 2D Representation of a laminar flow in a pipe

As said the diffusion accounting to the distribution of the additive takes place, even in the absence of fluid motion. Since we assume the fluid as isotropic, the diffusion will be constant and uniform. Therefore two independent processes shape the concentration profile: the additive´s diffusion and the fluid (motion or) *advection*. From this we define a *parameter p* expressing the relative contribution of these two processes. At this point it is particularly important to keep in mind the convenience of using *dimensionless* or *reduced* data, by forming the quotient from these two processes which then will free us from having to constantly specifying the physical units we´re working with whilst further enabling us to displaying the relative strength of the advection process over the diffusion, thus picturing a particular dominant tendency by a simple number. Therefore the said parameter *p* may vary between] 0, *a* [in our actual case; and is known in the literature as the *Péclet number*. The value *a,* a measure of the advection strength has a certain limit, because of the stated laminar case of the flow as we shall see in the next section explaining in detail the *Reynolds number,* and the *Péclet number.*

General observations and choice of the key-parameters

Dimensionless numbers play an important role in the process of reformulating the partial differential equations system: the incorporation of key-parameters and specifically dimensionless numbers enable for instance to predict or monitor the occurrence of a definite flow regime in a given range of *Reynolds* values; on the other hand key-parameters enable for instance fine-tuning upon *conditional occurrence* the resolution level to picture a flow regime transition.

Another important point worth mention is the role of key-parameters and dimensionless numbers in *dynamic similarity* enabling to replicate a model from lab-scale to real world applications or when translating a numerical model into an experiment. In those situations, detail-knowledge pertaining to the formulation of parameters, the scope of their use as well their re-scaling context will prove very helpful and should be consigned both in the experimental protocol and numerical Model documentation.

A perusal of today literature on hydrodynamics with thermodynamical processes shows there are currently about half hundred standard dimensionless numbers (and there will be more complex ones as we gain more

knowledge on complex flow physics and more sophisticated mathematical tools become available). Among these dimensionless numbers, the *Reynolds number* (abbreviated *Re*) and the *Péclet number (Pe)* are the most basic as they describe a given flow regime (laminar or turbulent) occurrence and the fundamentals of transport processes -pertaining to energy as well mass- in flow physics, respectively. Accordingly there are for instance *Pe* for mass transport and for energy transport.

Let us now examine *Pe* for mass transport defined as the ratio of the advection´s rate to the diffusion's rate:

$$Pe = \frac{LV}{D}; \quad (1), \text{ where}$$

- L is a representative (or reference) length,
- V a reference velocity,
- and D the mass diffusion´s coefficient.

The reference length L will depend on the geometry where the flow is being described. V in the case of a pressure gradient driven laminar flow through a pipe could be taken as the flow velocity along the tube axis. Moreover it could be assimilated to the maximum velocity under a given pressure gradient as shown in Figure1; and (L, d) a region of the tube where we´re interested in knowing the concentration profile; d being the tube diameter – in our 2D geometry the vertical distance between inner walls- und L the region´s length in the flow direction along the tube axis.

The *Reynolds number Re* is defined as the ratio of inertial forces to viscous forces. In the simple case of a flow through a pipe (Figure1), it is given as

$$Re = \frac{\rho VL}{\mu} = \frac{VL}{\nu}; \quad (2), \text{ where}$$

- ρ is the fluid density,
- V the mean fluid velocity,
- L a reference length as similarly defined in the case of *Pe,*
- μ the dynamic fluid viscosity (Pa.s),
- ν the kinematic viscosity (m^2 /s).

Turbulence occurs at high *Re* where dominant inertial forces induce instabilities leading to chaotic flow patterns, while low *Re* reflect the predominance of viscous forces which tend to streamline the velocity field. Therefore a laminar flow with diffusion process will have a *Pe* under a certain value determined by the maximum velocity as just stated at the end of the preceding section; the advection may indeed outweigh the diffusion process several orders of magnitude but the maximum velocity should lay below a critical value to keep the flow within the laminar regime limit: i.e. low *Re* typically below 2000 for a flow in a tube, according to standard experiments (see Ref [1]).

Having introduced the basic concepts, we want now to illustrate their application; to that effect we´ll consider another flow configuration requiring a reformulation of the given *Pe* in (1) to account for additional information: let us consider the case of hydrodynamic lubrication, where a fluid is squeezed between rotating co-axial cylinders c_1 and c_2 of opposite angular velocities: the fluid herein is subjected to shear stresses in such a way fluid layers adjacent to a given cylinder will be moved by shear forces in its own rotation direction. Additionally if their linear velocities are of equal absolute value, i.e. $\vec{v}_1 = -\vec{v}_2$; a shear gradient will progressively build up in such way half of the fluid will be pulled in one rotating direction and the other half by the cylinder rotating in the opposite direction. Since the shear forces, from geometric viewpoint, depend only on the linear velocities the system is then equivalent to a simpler shear flow between two parallel plates moving with the same velocity but in opposite directions, as shown in Figure2:

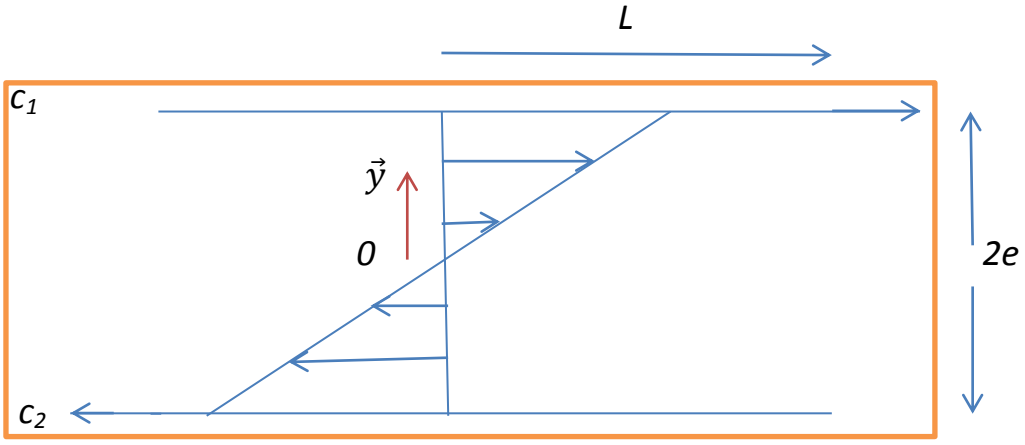

Figure2: shear flow between two parallel plates.

Let us further consider an additive, such as a dispersant injected (see $Note1$) into the fluid under these conditions and we are again interested in knowing the additive´s concentration profile: due to the symmetry we can limit ourselves to investigating the profile only in the (*L*, *e*) region. We therefore model the additive´s distribution through the following equation (see **Mathematical Annex**):

$$-\gamma\vec{y}.\vec{\nabla}n + D\nabla^2 n = \frac{\partial n}{\partial t}; \quad (3) \text{ , where}$$

- γ is the constant shear rate,
- $\vec{y}$ a variable running between 0 and e, the film thickness,
- $\vec{\nabla}n$ particles density gradient,
- D the diffusion constant,
- $\nabla^2 n$ the Laplace operator on particles density,
- $\frac{\partial n}{\partial t}$ the local variation of the particles density.

$Note1$

Oil additives are extensively used to maintain high oil viscosity values between surfaces in relative motion. To that effect VII (viscosity index improvers) consisting of larges molecule of chemical compounds are added. However due to service conditions those molecules are torn apart (see Ref.[2]) following shear stresses, causing the oil to thin down and possibly leak out; the torn apart VI Improvers then become contaminants which cause sludge if not removed. Under such conditions oil dispersants may be added to keep the contaminants in suspension (thus preventing sludge) until they are removed (within a reasonable time limit as lowered-viscosity oil film may induce detrimental heat surges between moving parts). I am inclined to believe this management policy may be particularly advantageous for critical industrial machines, such as isotopes separating centrifuges where up-time performance and running costs control are prime targets.

Before proceeding, we want to introduce some elements of dimensional analysis; to that effect we come back to the flow problem of the preceding section, where we stated we´ll prove the fully developed flow velocity field in the tube has a parabolic shape with maximum value at the center on the tube axis: let´s consider the system variables $\nabla P, V, \mu,$ and $y,$ where

- ∇P is the flow pressure gradient,
- V the velocity vector field,
- μ the dynamic viscosity, and

- y the variable running between 0 and d the distance between the plates as shown in Fig1.

We first construct the system-matrix SM whose columns consist of the variables and whose rows of the fundamental physical dimensions, namely the mass, time and length. Next we calculate the matrix K such that the product SM.K yields the null matrix. In linear algebra K is called the kernel of the system-matrix. The difference between the number of variables and the number of the fundamental physical dimensions involved represents the number of dimensionless groups, as stated by the Buckingham Pi theorem, (which is derived from the homogeneity requirements of equations with respect to the physical dimensions involved). In our case we've:

SM = $\begin{Bmatrix} 1 & 0 & 1 & 0 \\ -2 & 1 & -1 & 1 \\ -2 & -1 & -1 & 0 \end{Bmatrix}$; in our convention we´ve represented the variable *y* as the fourth matrix-column expressed in fundamental units of (mass, length, time) as $\begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix}$ and similarly ∇P [$ML^{-2}T^{-2}$] as the matrix-column $\begin{Bmatrix} 1 \\ -2 \\ -2 \end{Bmatrix}$.

- We therefore have 4-3= 1 Pi dimensionless Group and written as $\Pi = \nabla P^a V^b \mu^c y^d$; the exponents are the k-elements of the kernel matrix.

- We determine the matrix K such that SM.K= 0 i.e.

$$\begin{cases} -2a + b - c + d = 0 \\ -2a - b - c = 0 \\ a + c = 0 \end{cases}$$

Now solving the system with respect to one variable, say b, because we want to establish the relationship between V and the other variables yields:

$$\begin{cases} a = -b \\ c = b \\ d = -2b \end{cases}$$

That is $\Pi = \nabla P^{-b} V^b \mu^b y^{-2b}$; and since the constant Π can be expressed in power of b as C^b to make the equation homogeneous with respect to b, we get the simpler expression

$$V = C\frac{\nabla P}{\mu}y^2 \ . \quad (4)$$

Through the equation $V = C\frac{\nabla P}{\mu}y^2$ we´ve demonstrated that *V* is parabolic respectively to the variable y, running from 0 to d, the distance between the walls in our 2D-geometry. Now we show that V is symmetric around $d/2$, the tube axis, i.e. half-way between the walls: we first take note that V is null at both walls, because they are stationary; we therefore introduce two variables reflecting this symmetry, namely *+h/2* at $y = d$ and *-h/2* at $y = 0$*;* and further introduce the coordinate's transformation $y^2 \longrightarrow$ *Y²-(h/2)²:* the derivative $\frac{\partial V}{\partial Y}$ = $2C\frac{\nabla P}{\mu}Y$ is null at *0,* half-way between the plates and negative at *-h/2,* namely $-C\frac{\nabla P}{\mu}h$ and from *Y=0* positive and has growing values until *h/2 ;* namely $C\frac{\nabla P}{\mu}h$*,* the opposite value *at –h/2.* Therefore the flow velocity field *V* is symmetric and layered around the tube axis (or half-way between the walls in our 2D-geometry).

Correction

The derivative $\frac{\partial V}{\partial Y}$ = $2C\frac{\nabla P}{\mu}Y$ is indeed null at $Y = 0$ and therefore any value λ yielding $2C\frac{\nabla P}{\mu}\lambda$ will have its opposite derivative value $-2C\frac{\nabla P}{\mu}\lambda$ at its equidistant opposite $-\lambda$; not just $\pm h/2$. Therefore the profile is symmetric and layered around $Y = 0$. However the equation (4) doesn´t give justice to the fact $V(y = 0) = V(y = d) = 0$, due to friction which cause the flow layers in close contact with the walls to halt. This shortcoming stems from the fact that we did not integrate in the formulation of our SM this additional boundary conditions requirement. It should be noted, this requirement is a physical one, not the result of any mathematical constraint. We therefore introduce a further dimensionless group $\Pi_2 = \frac{y}{d}$; and since any dimensionless group can be re-expressed as a combination of the remaining group-subset, we write $\Pi = f(\Pi_2)$, i.e.

$\Pi = f\left(\frac{y}{d}\right)$. We therefore rewrite (4) as

$V = C\frac{\nabla P}{\mu}\frac{y^2}{d^2} + K\frac{y}{d}$; (i.e. from a parabola having the expression ax^2 , to ax^2 +bx after substitution). The coefficient K will be determined by the boundary condition $V(y = d) = 0$ giving

$K = -C\frac{\nabla P}{\mu}$. Therefore

$$V = C\frac{\nabla P}{\mu}\left(\frac{y^2}{d^2} - \frac{y}{d}\right). \quad (5)$$

.

Similarly we first apply Dimensional Analysis to equation (3) to find out possible dimensionless groups: our variables are $\gamma, D, z;$ where $0 < z < y$ (see Figure2) is used to define a region z^2 having a relaxation-time τ. We further introduce the element of viscosity μ to account for realer situations: the system-matrix is then

$\underline{\underline{SM}} = \begin{Bmatrix} 0 & 0 & 0 & 1 \\ 0 & 2 & 1 & -1 \\ -1 & -1 & 0 & -1 \end{Bmatrix}$; solving $\underline{\underline{SM}}.\underline{K} = \underline{0}$ yields the kernel:

$\underline{K} = \begin{Bmatrix} d = 0 \\ b = -a \\ c = 2a \end{Bmatrix}$ for the Pi Group $\Pi = \gamma^a D^{-a} z^{2a} \mu^0$ gives $C = \frac{\gamma z^2}{D}$; which is the ratio of the shear rate advection to the diffusion rate, i.e. the *Pe* for our flow configuration. Therefore $Pe = \frac{\gamma z^2}{D}$. (6)

Substituting into (3) and introducing h^2 as the quadratic grid mesh unit (see legend Figure3) in the discretized *(x, y)* Plane gives

$$-\frac{Pe}{NM} j\nabla^0 n + \Delta^0 n = \frac{\partial n}{\partial t^0}\frac{\tau_D}{t_{ref}} \; ; \quad (6a) \text{ , where}$$

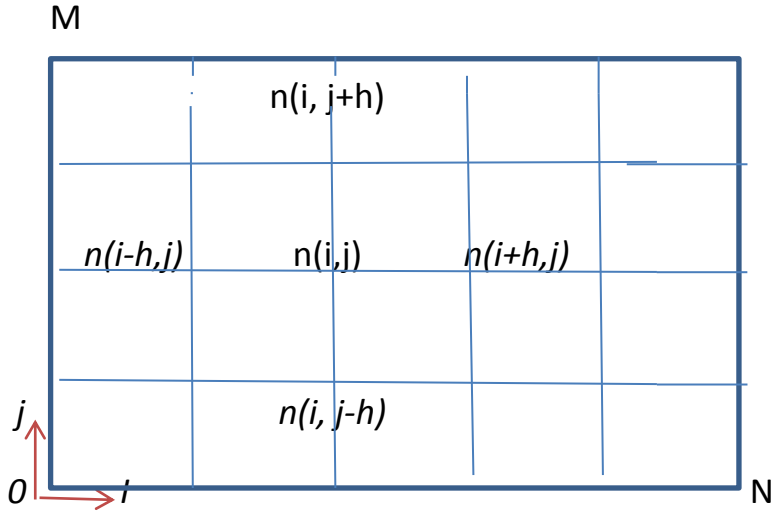

Figure3: Discretization of the (MN) Plane with *0 < i < N* and *0< j < M* on a quadratic grid of mesh unit h^2 , *i = j = h.*

- $j = \frac{y}{h}$; and t_{ref} a resolution-level factor which shall be explained in the section **"Introduction of additional parameters as appropriate".**
- $\nabla^0 n$ the dimensionless gradient $\nabla^0 n = h\nabla n$; and similarly
- $\Delta^0 n = h^2 \nabla^2 n$ the dimensionless divergence of the particles density gradient:

  $$\Delta^0 n = \sum_{K=1}^{4} n_K - 4n(i,j); \quad (7)$$

  where the n_K are the 4 grid points $n(i \pm h, j \pm h)$ around *n(i, j)* as shown in Figure3. A demonstration of the equation (7) as well the derivation of the expression of the dimensionless gradient will be presented in the **Mathematical Annex**.
- τ_D diffusion time expressed as function of *h* and *D*: $\tau_D = \frac{h^2}{D}$ (8)
- τ_{rl} a relaxation time over the region *(MN)* following a given shear rate application:

  $$\tau_{rl} = \tau_D \text{ (MN)} ; \quad (9)$$

- $\frac{\partial n}{\partial t^0}$ the dimensionless local particles density variation with respect to $\frac{\tau_D}{t_{ref}}$. In the C-Program implementing the numerical approximation, the expression $\frac{\partial n}{\partial t^0} \frac{\tau_D}{t_{ref}}$ is substituted by $\frac{n(t+1)^k - n(t)^{k-1}}{RES}$; the superscript *k* denotes the k^{th} iteration and *RES* a variable expressing the resolution-level in function of the shear rate strength γ (expressed in terms of the Pe), the reference time t_{ref} and the relaxation time τ_{rl}.

The section **"Introduction of additional parameters as appropriate"** will give ample details on the motivation for introducing the variable *RES* alongside its arguments t_{ref} , τ_{rl} and Pe.