DERIVATION OF THE EQUATIONS OF MASS TRANSFER WITH RETENTION AND THE KORTEWEG-DEVRIES EQUATION

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Abstract. *It is shown that the one dimensional mass transfer with temporary retention in the positive x-direction may be dealt with a simple discrete model. From the clues provided by the discrete approach, particularly those concerning the need to introduce a third order differential term and appropriate control parameters to define the validation range of the model, it is possible to propose the kinematic laws governing the mass transfer phenomenon with temporary retention for a continuum system. Two types of excitation states, one characterized by the linear momentum and the other by the angular momentum, are introduce for the derivation of the kinematic laws associated to the continuum system. Mass conservation princple is used to derive the governing equations. The resulting governing equation is of the Korteweg-deVries type. A brief discussion about the governing equation and its similarity with the classical Korteweg-deVries equation is presented.The kinematic laws introduced show clearly that the solution must belong to the class of dispersive waves.*

Keyword:s *mass transport, temporary retention, Korteweg-deVries equation, dispersive wave, discrete approach.*

1. INTRODUCTION

The classical discrete approach to the one-dimensional mass transfer problem in the positive x-direction after taking the appropriated limits leads to the classical first order wave equation. The retention of a fraction of the moving particles is usually ignored. Differently from the dissipation problem where retention may be important in several engineering applications, as far as we know retention associated to wave motion has not deserved enough attention of engineers and scientists.

This fact may be credited to the difficulty in establishing a consistent law for the retention effect and maybe to the lack of important applications. The formulation of a law for the continuum case is indeed difficult, but it can be successfully attained if we use the clues given by a relatively easy discrete formulation.

We will see that within certain hypotheses that are not too restrictive the formulation of a temporary retention law may be proposed. The physical requirements for the theory to be valid may consider some idealized conditions as energy conservation and two particular excitation states of the particles involved in the motion. As a matter of fact physic-chemical laws at intermediate scales always require some idealization of the dynamical process. In general the physic-chemical laws assume average values for the parameters controlling the main variables assumed to play the major roles in the process. In other words a law in physics, chemistry or engineering is a fundamental tool to assemble a model that is supposed to simulate satisfactorily the real world. Validation of the model will determine the range of the response for which the theory is applicable.

In the next sections we will develop the formulation of the mass transfer problem with retention first with a discrete approach and then for a continuum with the help of a transfer law and a retention law.

The control parameters appearing as a logical condition from the deduction of the discrete approach are remarkable for they provide the admissible variation range of the coefficients of the differential terms in the governing equation for the model to be valid. Depending on the trapped fraction of the particles the model covers the different dynamical processes from the classical first order wave equation – no retention – till the stationary case where all particles will be eventually trapped – full retention. These control parameters are kept in the continuum approach and are essential for the formulation of the laws governing the process. Without the clue provided by the discrete approach it would be very hard to find the form of the control parameters.

The governing equation of mass transfer with retention obtained here for a given non-homogeneous medium is similar to the Koertweg-deVries equation (Jager, 2006, Lighthill,1978, Whitham, 1974,) except for the sign of the third order differential term. Despite this small difference the behavior of the solutions might be quite different. The dispersion relation for the mass transfer with retention is derived and discussed briefly for the case of the linearized equation.

2. THE DISCRETE FORMULATION.

Consider the distribution law that combines partial retention with mass transfer in the x-positive direction. Suppose that a fraction k<1 of the initial mass in the cell n is transferred to the cell n+1 located next to the cell n to the right. The exceeding fraction (1-k) of the mass remains temporarily retained in the cell n. Clearly the motion has a preferred direction as indicated by the arrows in the Fig. 1 and the mass of a given cell is partially transferred to the neighbor cell.

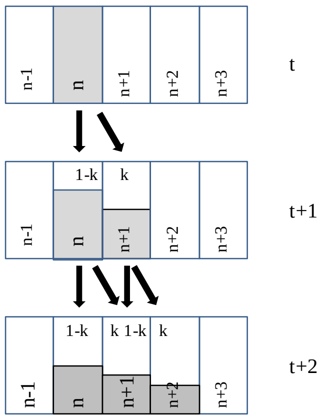

Fig.1. Evolution of the mass profile for propagation in the x-positive direction with partial retention.

The analytical expressions of this law are easily written:

$$p_n^{t+1} = (1-k)\,p_n^t + k p_{n-1}^t \qquad (1\text{-a})$$

$$p_n^{t} = (1-k)\,p_n^{t-1} + k p_{n-1}^{t-1} \qquad (1\text{-b})$$

$$p_n^{t-1} = (1-k)\,p_n^{t-2} + k p_{n-1}^{t-2} \qquad (1\text{-c})$$

Where $0 \le k \le 1$. In order to keep the correct response for the intermediate steps for all values of the parameter k it is necessary to take double time step (t+1) and (t-1) for the calculation of the difference in time, that is, the calculations will be carried out with the difference $\left(p_n^{t+1} - p_n^{t-1}\right)$. After a sequence of algebraic operations, as shown in the appendix A, we arrive at the following equation (A-5):

$$\left[\frac{\Delta p_n^t}{\Delta t} + \frac{\mathrm{O}(\Delta t)^2}{\Delta t}\right]\Delta t = k\left\{\left[\frac{(1-k)}{2}\frac{\Delta^3 p_n}{\Delta x^3} + \frac{\mathrm{O}(\Delta x)^4}{\Delta x^3}\right]\Delta x^3 - \left[\frac{\Delta p_n}{\Delta x} + \frac{\mathrm{O}(\Delta x)^2}{\Delta x}\right]\Delta x\right\}^{t-2\Delta t}$$

Again this expression satisfies the conditions required for k=0 and k=1.Now let us define:

$$\frac{\Delta x}{\Delta t} = \frac{L_0}{m}\frac{m}{T_0} = \frac{L_0}{T_0}$$

$$\frac{\Delta x^3}{\Delta t} = \left(\frac{L_1}{m^{1/3}}\right)^3 \frac{m}{T_0} = \frac{L_1^3}{T_0}$$

where L_0, L_1 and T_0 are scale factors, $\Delta x = L_0/m = L_1/m^{1/3}$ and $\Delta t = T_0/m$ are increment size and time interval respectively. Substituting the above relations in the finite difference equation and taking the limits $\Delta x \to 0, \Delta t \to 0$ we get:

$$\frac{\partial p}{\partial t} = \frac{1}{2}\frac{L_1^3}{T_0}k(1-k)\frac{\partial^3 p}{\partial x^3} - \frac{L_0}{T_0}k\frac{\partial p}{\partial x}$$

Taking the proper limits and defining $K_1 = L_0/T_0$ and $K_3 = L_1^3/T_0$ we finally get:

$$\frac{\partial p}{\partial t} = K_3 k(1-k)\frac{\partial^3 p}{\partial x^3} - K_1 k \frac{\partial p}{\partial x} \tag{2}$$

Clearly the equation (2) satisfies the mechanical requirements imposed by the parameter k. For k=0 the solution is stationary and for k=1 the solution falls in the category of a travelling wave. As in the previous problems keeping the control parameters explicitly in the equation is helpful even for a continuum formulation.

It is remarkable the presence of the third order derivative in the equation of propagation with temporary retention. This term is required if temporary retention is to be taken into account. The derivation of a constitutive law for this kind of phenomenon starting from the generalized analysis of a continuum is a difficult task. The clue given by the discrete approach is fundamental to develop a consistent constitutive law.

3. THE CONTINUUM FORMULATION

The discrete approach suggests that the unidirectional transport of a bulk of particles with temporary and partial retention needs to incorporate a third order differential term in the governing equation. We will assume this condition as a milestone of the theory for the continuum problem. Besides, the control parameters multiplying the third and first order terms must be retained in the continuum formulation since they define precisely the limits of transport without retention k=1 and the steady state k=0. The parameter k as seen previously may vary within the interval [0,1]. Therefore we state as a fundamental axiom:

Proposition 1. The governing equation for unidirectional mass transportation with retention must contain the term

$$K_3 k \frac{\partial^3 p(x,t)}{\partial x^3}$$

where p(x,t) is the variable representing mass concentration, K_3 is a material constant and $k \in [0,1]$.

This axiom requiring the insertion of the third order term in the governing equation will provide the fundamental clue and direction to formulate the laws of motion. Consider two fundamental motions, namely, a translational motion with velocity v and a circulatory motion along a closed trajectory with a small radius δ and angular velocity ω. The circulatory motion may degenerate into a spin. Any particle may be excited by a combination of a translational motion and a circulatory motion moving along a spiral trajectory, a kind of vortex. The kinematic state of a particle with mass m corresponding to the translational motion is characterized by the kinetic energy $E_T = p^2/2m$ where p is the linear momentum $p=mv$, and the kinematic state corresponding to the circulatory motion is characterized by the kinetic energy $E_R=L^2/2I$ where L is the angular momentum $L=m\delta^2\omega$ (or $L=I\,\omega$ for the case of a spin).

Now let us consider two fundamental kinematic states, namely;

I. A particle belongs to the **state I** if it follows a straight trajectory in the x-positive direction with translational energy E_T much larger than the rotational energy E_R. That is $v >> \delta\omega$.

II. A particle belongs to the **state II** if the rotational energy E_R is much larger than the translational energy E_T. That is $\omega >> v/\delta$. A particle in this state moves backwards at a very low speed.

We will assume that a given particle may jump from **state I** into **state II** and vice-versa when excited by some cause such that all particles will be moving and the total kinetic energy will be kept approximately constant. Moreover a particle cannot be trapped permanently, that is subtracted from the process since this would mean a kind of sink that belongs to a different class of problems. The exchange of states may be credited to particles interaction with the supporting medium for instance. We assume here that all particles are either in **state I** or in **state II**. Under this assumption the mass conservation principle reads:

$$\frac{\partial}{\partial t}\int_V p(x,t)dV + \int_{\partial V} \mathbf{U.n} dS = 0 \tag{3}$$

where $p(x,t)$ is the specific mass, V is an elementary volume, **U** is the net flux of particles across the boundary surface ∂V and **n** is the unit vector normal to ∂V. The flux vector **U** may be decomposed into two components representing the particles in the **state I** and in the **state II**. If we call k the fraction of particles in **state I** and (*1-k*) the fraction of particles in the **state II** we may write:

$$\mathbf{U} = k\mathbf{U}_I - (1-k)\mathbf{U}_{II} \tag{4}$$

where $\mathbf{U}_I$ and $\mathbf{U}_{II}$ represent the mass flux of the particles in **state I** and in **state II** respectively. Note that the velocity of particles in the **state II** has a negative sign due to the initial assumption that they move backwards. Introducing equation (4) into equation (3) we get:

$$\frac{\partial}{\partial t}\int_V p(x,t)dV + \int_{\partial V}(k\mathbf{U}_I - (1-k)\mathbf{U}_{II}).\mathbf{n}dS = 0 \tag{5}$$

Now we need to introduce the constitutive relations for the continuous forward flow and for the backwards flow. The backwards flow is assumed to be very slow since almost all the kinetic energy is transferred to the circulatory motion. Therefore we may say that the (*1-k*) particle fraction is temporarily retained in a thin boundary layer in the neighborhood of the boundary surface ∂V. The first law that we may propose concerns the predominant forward motion:

First law. *The mass flux across the boundary surface ∂V corresponding to the particles in the kinematic **state I** is proportional to the mass concentration p(x,t):*

$$\mathbf{U}_1 = c_0 p(x,t)\vec{e}_1 \tag{6}$$

where c_0 is the speed of propagation of the mass fraction k in the x-positive direction.

The corresponding physical meaning clearly expresses that the particle speed in the **state I** is independent of the mass fraction moving forward. For any mass fraction moving forward the speed is the same as the classical wave equation for full forward motion without retention c_0 :

$$\frac{\partial p}{\partial t} + c_0\frac{\partial p}{\partial x} = 0$$

Therefore equation (6) is equally valid for the motion with and without retention. The second law dealing with particles in the kinematic **state II** is more complex and may be stated as follows:

Second law. *Let* $\boldsymbol{\psi}$ *be a vector parallel to the direction of motion proportional to the mass concentration:*

$$\boldsymbol{\psi} = bp(x,t)\vec{e}_1$$

The parameter b is a material constant depending on the nature of the particles and the supporting medium. Define the blocking effect B as the divergent of the vector $\boldsymbol{\psi}$*:*

$$B = div\boldsymbol{\psi} = \frac{\partial}{\partial x}(bp(x,t))$$

*The retention effect or the ideal mass flux through the boundary surface ∂V corresponding to the particles in the kinematic **state II** is defined by a vector proportional to the gradient of B multiplied by the particle fraction moving forward, that is:*

$$\mathbf{U}_{II} = \hat{r}k\frac{\partial^2}{\partial x^2}(bp(x,t))\vec{e}_1$$

The parameter $\hat{r}$ is a material constant depending on the nature of the particles and the supporting medium.

Note that the retention effect exists only if there are particles moving forward, $k > 0$, that is, if the wave front is moving forward. Retention only doesn't exist. For sake of simplicity and due to the lack of experimental results we will assume here b=constant and introduce a material constant $r = b\hat{r}$ combining b and $\hat{r}$. Introducing the above results in the equation (3) it is immediately obtained:

$$\frac{\partial}{\partial t}\int_V p(x,t)dV + \int_{\partial V}\left[kc_0 p(x,t) - (1-k)rk\frac{\partial^2 p(x,t)}{\partial x^2}\right]\vec{e}_1.\mathbf{n}dS = 0$$

For $p(x,t)$ sufficiently smooth the Green´s theorem gives:

$$\int_V\left[\frac{\partial p(x,t)}{\partial t} + div\left(kc_0 p(x,t) - (1-k)rk\frac{\partial^2 p(x,t)}{\partial x^2}\right)\right]dV = 0$$

And since V is arbitrary we finally get:

$$\frac{\partial p(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(kc_0 p(x,t) - (1-k)rk\frac{\partial^2 p(x,t)}{\partial x^2}\right) = 0 \tag{7}$$

For c_0 , r and k constants we have:

$$\frac{\partial p(x,t)}{\partial t} + c_0 k\frac{\partial p(x,t)}{\partial x} - rk(1-k)\frac{\partial^3 p(x,t)}{\partial x^3} = 0 \tag{8}$$

Equation (8) reproduces the equation (2) with $K_1=c_0$ and $K_3=r$. In general however the parameters r and c_0 may be functions o x for a non-homogeneous medium. More critical is the parameter k that in general may be expected to be a function of temperature and other thermodynamical variables. It is also possible that $k=k(p)/\mathrm{k}_0$ where $k_0 = k(p_0)$ meaning that retention saturates for $p = p_0$. For this case the governing equation becomes non-linear and the solution may be very hard to be found even for homogeneous media.

Now suppose that the process takes place in a non homogeneous medium, such that:

$$c_0 = c_1 - \frac{1}{2}c_2 p$$

That is the speed of mass transfer (wave speed) when retention is turned off is a linear function of the concentration $p(x,t)$ increasing when the concentration decreases. That is the wave speed is higher in rarefied regions. Suppose that the other parameters are constants. Equation (7) then reads:

$$\frac{\partial p(x,t)}{\partial t} + k(c_1 - c_2 p(x,t))\frac{\partial p(x,t)}{\partial x} - (1-k)rk\frac{\partial^3 p(x,t)}{\partial x^3} = 0$$

With $q(x,t) = c_1 - \frac{1}{2}c_2 p(x,t)$ we have:

$$\frac{\partial q(x,t)}{\partial t} + kq(x,t)\frac{\partial q(x,t)}{\partial x} - (1-k)rk\frac{\partial^3 q(x,t)}{\partial x^3} = 0 \tag{9}$$

Equation (9) is a modified form of the KdV equation. Since $0 \le k \le 1$ and r is positive the coefficient of the third order derivative is always negative and therefore it differs from the original KdV equation. This detail will certainly introduce drastic differences in the qualitative behavior of the solution. The redistribution law of the mass transport in the x-positive direction strongly suggests the formation of backscattering in the course of the evolution process.

4. FINAL REMARKS

It is remarkable that with a relatively simple procedure, taking the limit of a discrete approach, it is possible to show that the governing equation for one-dimensional mass transfer in the positive x-direction with retention requires a third order differential term. The resulting equation is a third order equation linear equation similar to the linearized Kordeveg deVries equation. A fundamental difference however, namely the sign of the coefficient of the third derivative, may introduce substantial differences between the respective solutions. Indeed if we take a perturbation of the type:

$$\varsigma(x,t) = \varsigma_0 \exp\left(\frac{i}{\lambda}(x-ct)\right)$$

and introduce in a linearized KdV :

$$u_t + c_0 u_x + \sigma u_{xxx} = 0$$

where $\sigma = c_0 h^2/6$ the following dispersion relation is readily obtained:

$$\frac{c}{c_0} = \left(1 - \frac{1}{6}\left(\frac{h}{\lambda}\right)^2\right)$$

For the case of equation (8) the dispersion relation is:

$$\frac{c}{c_0} = k(1+(1-k)\varepsilon) \qquad 0 \leq k \leq 1 \quad \text{and} \quad \varepsilon = r/\lambda^2 c_0$$

The dispersion relation for the KdV equation applies for relatively long waves as compared with the shallow water depth, that is when $\lambda >> h$, so that the wave speed is positive. The dispersion relation for the case of mass transfer with retention has no restriction in principle. As shown in the Fig.2 if k=1 the wave speed is reduced to c_0

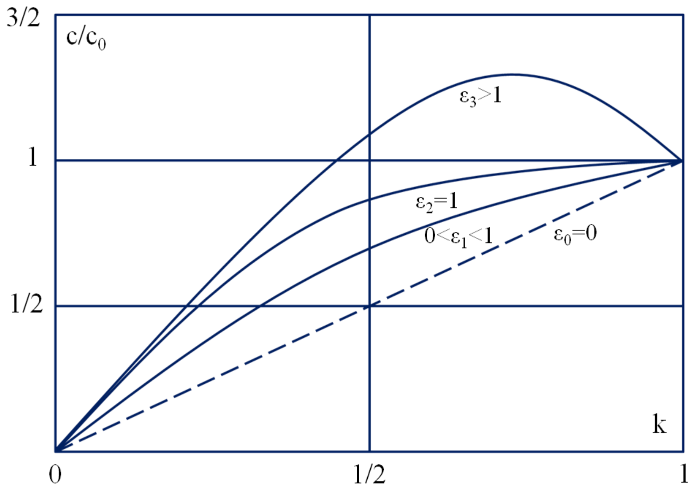

Figure 2. Dispersion relation for the mass transfer problem as function of the mass fraction k moving forward for different values of the parameter $\varepsilon = r/\lambda^2 c_0$. Dashed curve represents the limiting case where $\varepsilon \rightarrow 0$. For ε=1the curve reaches a maximum at k=1.

representing the speed corresponding to the classical problem with no retention. If k=0 there is no motion the solution is stationary. Note that the dispersion relation returns always a positive wave speed. For very long waves the wave speed is given by $c \approx kc_0$ and is reduced to a linear function of the mass fraction k moving ahead.

For ε=1 the dispersion relation reaches a maximum at k=1. For very short waves ε >1 the dispersion relation leads to wave speeds higher than c_0 for certain values of the mass fraction moving in the x-positive direction. The maximum value of c for those cases falls in the range 1/2 < k < 1. This means that the retention in the presence of very short waves may introduce wave velocities higher than c_0 and short waves could catch up long waves inducing possibly the formation of shock fronts.

The solution of the equations presented above need to be carefully explored. Due to the difference in sign of the third order differential term as compared with the KdV equation it is not possible to adopt the solutions already available for this last equation (Miura, 1967, Soliman, 2006, Bhatta and Bahtti, 2006, Chunxiong et all) without a detailed analysis. While for the linearized KdV equation long waves move faster than short waves for the case of propagation with retention short waves are speed dominant moving faster than long waves. Also the fact that the dispersion relation has a maximum within the range of valid solutions is a critical difference from the classical case of the linearized KdV equation. Figure 3 presents a sketch of the expected results for the dispersion relations for propagation with retention and for the linearized KdV. Note that for the KdV equation the relation c/c_0 holds only

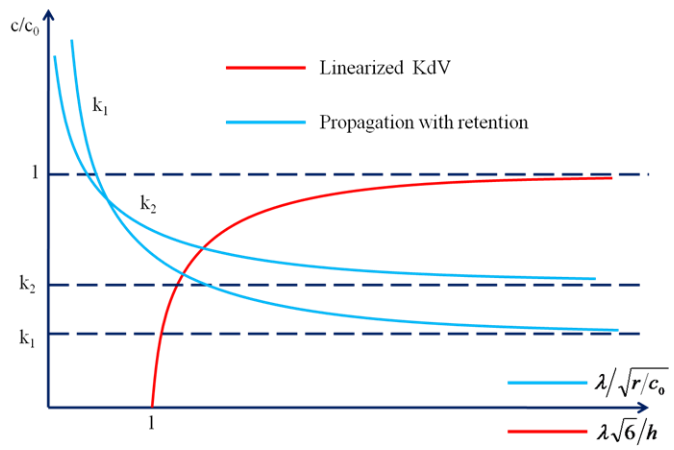

Figure 3. Dispersion relation for the linearized KdV equation and for the equation of propagation with retention as function of the wave length.

for long waves, $\lambda\sqrt{6}/h > 1$ while for propagation with retention there is no restriction in principle. The relation c/c_0 is limited below by the correspondent moving fraction k as mentioned before leading to $c \approx kc_0$ for very long waves as shown in the Fig.3. Two curves for different fractions k_i and k_j , i $\neq$ j, intercept at $\lambda/\sqrt{r/c_0} = \sqrt{k_i + k_j - 1}$ for all $k_i + k_j > 1$. Given that $k_i + k_j < 2$ the locus of intersection of all curves k_i falls within the interval $0 < \lambda/\sqrt{r/c_0} < 1$. The dependence of the dispersion relation on λ is substantially different for both cases which indicate that in general the respective solutions will probably present quite diverse behavior. For very long waves however asymptotic expansion of the respective solutions may present similar behavior. We leave the discussion on the analytical and numerical solutions of the equations for mass transfer with retention for a next paper.

Finally we believe that experimental setups are not difficult to devise introducing appropriated devices that could transform linear momentum into angular momentum for some fraction of the particles moving in the positive x-direction with a minimum of dissipation. Unfortunately we were not able to find references to similar problems in the current literature. A recent paper on the behavior of mass transfer among black holes [Holley-Bockelmann et all] mention this kind of problem but the approach adopted is quite different from the formulation presented here. Another interesting reference dealing with backscattering of ballistic electrons constrained to move in a corrugated surface topography [Sotomayor et all] introduces a similar problem that is modeled with quite different equations.

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6. RESPONSIBILITY NOTICE

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APPENDIX A

One dimensional propagation with retention.

The rule to be followed for this particular case reads:

$$p_n^{t+1} = (1-k)\,p_n^t + kp_{n-1}^t \qquad \text{(A-1a)}$$
$$p_n^t = (1-k)\,p_n^{t-1} + kp_{n-1}^{t-1} \qquad \text{(A-1b)}$$
$$p_n^{t-1} = (1-k)\,p_n^{t-2} + kp_{n-1}^{t-2} \qquad \text{(A-1c)}$$

For $0 \le k \le 1$. Using the same procedure as before, and performing the tests for the critical values of k, the following results are obtained successively:

$$\begin{aligned} p_n^{t+1} - p_n^{t-1} &= \left[(1-k)p_n^t + kp_{n-1}^t\right] - \left[(1-k)p_n^{t-2} + kp_{n-1}^{t-2}\right] = \\ &= \left\{(1-k)\left[(1-k)p_n^{t-1} + kp_{n-1}^{t-1}\right] + k\left[(1-k)p_{n-1}^{t-1} + kp_{n-2}^{t-1}\right]\right\} - \left[(1-k)\,p_n^{t-2} + kp_{n-1}^{t-2}\right] \end{aligned} \qquad \text{(A-2)}$$

Now considering the function $p(x,t)$ sufficiently regular we may write:

$$p_n^{t+1} - p_n^{t-1} = \left(p_n^{t+1} - p_n^t\right) + \left(p_n^t - p_n^{t-1}\right) = 2\left(p_n^{t+1} - p_n^t\right) + \mathrm{O}(\Delta t)^2$$

Introduce this expression in (A-2) and rearrange the terms to obtain:

$$\begin{aligned} 2\left(p_n^{t+1} - p_n^t\right) + \mathrm{O}(\Delta t)^2 &= \left[(1-k)^2 p_n^{t-1} + 2k(1-k)p_{n-1}^{t-1} + k^2 p_{n-2}^{t-1}\right] - \left[(1-k)p_n^{t-2} + kp_{n-1}^{t-2}\right] = \\ &= \left[(1-k)^2\left((1-k)p_n^{t-2} + kp_{n-1}^{t-2}\right) + 2k(1-k)\left((1-k)p_{n-1}^{t-2} + kp_{n-2}^{t-1}\right) + k^2\left((1-k)p_{n-2}^{t-2} + kp_{n-3}^{t-2}\right)\right] - \\ &- \left[(1-k)p_n^{t-2} + kp_{n-1}^{t-2}\right] \end{aligned}$$

Or

$$2\left(p_n^{t+1}-p_n^t\right)+\mathrm{O}(\Delta t)^2=(1-k)^3p_n^{t-2}+3k(1-k)^2p_{n-1}^{t-2}+3k^2(1-k)p_{n-2}^{t-2}+k^3p_{n-3}^{t-2}-$$
$$-(1-k)p_n^{t-2}-kp_{n-1}^{t-2}$$

Clearly for k=0, $\left(p_n^{t+1}-p_n^t\right)=0$ except for terms of higher order, that is, we arrive at a stationary solution matching the results obtained with equations (A-1a,b,c). For k=1 the right hand side term reads $\left(p_{n-3}^{t-2}-p_{n-1}^{t-2}\right)$. Now considering the function $p(x,t)$ sufficiently regular we may write:

$$p_{n-3}^{t-2}-p_{n-1}^{t-2}=-\left(p_{n-2}^{t-2}-p_{n-3}^{t-2}\right)-\left(p_{n-1}^{t-2}-p_{n-2}^{t-2}\right)=-2\left(p_n^{t-2}-p_{n-1}^{t-2}\right)-\mathrm{O}(\Delta x)^2$$

Therefore for k = 1 we have:

$$2\left(p_n^{t+1}-p_n^t\right)+\mathrm{O}(\Delta t)^2=-2\left(p_n^{t-2}-p_{n-1}^{t-2}\right)+\mathrm{O}(\Delta x)^2$$

The left hand side term means variation with respect to t and the right hand side term means variation with respect to x. Therefore except for terms of higher order the above expression indicates propagation exactly as required. Continuing with the algebraic manipulation we get:

$$2\left(p_n^{t+1}-p_n^t\right)+\mathrm{O}(\Delta t)^2=k(1-k)(-2+k)p_n^{t-2}+k\left(2-6k+3k^2\right)p_{n-1}^{t-2}++3k^2(1-k)p_{n-2}^{t-2}+k^3p_{n-3}^{t-2}$$

or

$$2\left(p_n^{t+1}-p_n^t\right)+\mathrm{O}(\Delta t)=k\left\{(1-k)\left(-2p_n^{t-2}+kp_n^{t-2}+3kp_{n-2}^{t-2}\right)+k\left(2-6k+3k^2\right)p_{n-1}^{t-2}+k^3p_{n-3}^{t-2}\right\} \quad (\mathrm{A-3})$$

Noting that:

$$\left(-2p_n^{t-2}+kp_n^{t-2}+3p_{n-2}^{t-2}\right)=-2p_n^{t-2}+k\left(p_n^{t-2}-3p_{n-1}^{t-2}+3p_{n-2}^{t-2}-p_{n-3}^{t-2}\right)+k\left(3p_{n-1}^{t-2}+p_{n-3}^{t-2}\right)=$$
$$=-2p_n^{t-2}+k\Delta^3p_n^{t-2}+\mathrm{O}(\Delta x)^4+k\left(3p_{n-1}^{t-2}+p_{n-3}^{t-2}\right)$$

and introducing this expression in (A-3) we get successively:

$$2\left(p_n^{t+1}-p_n^t\right)+\mathrm{O}(\Delta t)^2=k(1-k)\Delta^3p_n^{t-2}+\mathrm{O}(\Delta x)^4+k(1-k)\left[-2p_n^{t-2}+3kp_{n-1}^{t-2}+kp_{n-3}^{t-2}\right]+$$
$$+k\left[2-6k+3k^2\right]p_{n-1}^{t-2}+k^3p_{n-3}^{t-2}$$

$$2\left(p_n^{t-1}-p_n^t\right)+\mathrm{O}(\Delta t)^2=k(1-k)\Delta^3p_n^{t-2}+\mathrm{O}(\Delta x)^4+$$
$$+k\left\{-2p_n^{t-2}+3kp_{n-1}^{t-2}+kp_{n-3}^{t-2}+2kp_n^{t-2}-3k^2p_{n-1}^{t-2}-k^2p_{n-3}^{t-2}\right\}+$$
$$+k\left\{2p_{n-1}^{t-2}-6kp_{n-1}^{t-2}+3k^2p_{n-1}^{t-2}+k^2p_{n-3}^{t-2}\right\}$$

$$2\left(p_n^{t+1}-p_n^t\right)+\mathrm{O}(\Delta t)^2=k(1-k)\Delta^3p_n^{t-2\Delta t}+\mathrm{O}(\Delta x)^4+$$
$$k\left\{+kp_{n-3}^{t-2}+2kp_n^{t-2}-3kp_{n-1}^{t-2}+2p_{n-1}^{t-2}-2p_n^{t-2}\right\} \quad (\mathrm{A-4})$$

Performing again the test for k we obtain, for k=0, $\left(p_n^{t+1}-p_n^t\right)=0$ stationary solution as required and for k=1, $2\left(p_n^{t+1}-p_n^t\right)+\mathrm{O}(\Delta t)^2=-2\left(p_n^{t-2}-p_{n-1}^{t-2}\right)+\mathrm{O}(\Delta x)^2$ propagation solution as required. Rearranging the terms of (A-4) we get:

$$\left(p_n^{t+1} - p_n^t\right) + \mathrm{O}(\Delta t)^2 = \frac{k(1-k)}{2}\Delta^3 p_n^{t-2\Delta t} + \frac{k}{2}\left\{2(1-k)\left(p_{n-1}^{t-2} - p_n^{t-2}\right) + k\left(p_{n-3}^{t-2} - p_{n-1}^{t-2}\right)\right\}$$

Recalling that $\left(p_{n-1}^{t-2} - p_n^{t-2}\right) = -\Delta p_n^{t-2}$ and $\left(p_{n-3}^{t-2} - p_{n-1}^{t-2}\right) = -2\Delta p_n^{t-2} + \mathrm{O}(\Delta x)^2$ we may write:

$$\left(p_n^{t+1} - p_n^t\right) + \mathrm{O}(\Delta t)^2 = \left\{\frac{k(1-k)}{2}\Delta^3 p_n + \mathrm{O}(\Delta x)^4 + \frac{k}{2}\left[-2(1-k)\Delta p_n - 2k\Delta p_n + \mathrm{O}(\Delta x)^2\right]\right\}^{t-2\Delta t}$$

$$\Delta p_n^t + \mathrm{O}(\Delta t)^2 = \left\{\frac{k(1-k)}{2}\Delta^3 p_n + \mathrm{O}(\Delta x)^4 - k\Delta p_n + \mathrm{O}(\Delta x)^2\right\}^{t-2\Delta t}$$

Again this expression satisfies the conditions required for k=0 and k=1. The differential form is then obtained:

$$\left[\frac{\Delta p_n^t}{\Delta t} + \frac{\mathrm{O}(\Delta t)^2}{\Delta t}\right]\Delta t = k\left\{\left[\frac{(1-k)}{2}\frac{\Delta^3 p_n}{\Delta x^3} + \frac{\mathrm{O}(\Delta x)^4}{\Delta x^3}\right]\Delta x^3 - \left[\frac{\Delta p_n}{\Delta x} + \frac{\mathrm{O}(\Delta x)^2}{\Delta x}\right]\Delta x\right\}^{t-2\Delta t} \qquad \text{(A - 5)}$$