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Transformation of a given PDE to a DAE using the Orthogonal Collocation Method on Finite Elements

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1 Introduction

In this document, we discuss how to transform the PDE used to model a 1-D clarifier [1] (which forms part of a waste water treatment plant) into a differential algebraic equation (DAE). We use the PDE to look at two test case conditions for the clarifier: continuous and batch sedimentation [2].

We use z to represent the coordinate along the length of the 1-D clarifier. The top and bottom ends of the clarifier are located at $z = 0$ and $z = L$ respectively. As discussed in detail in [2], the PDEs for both test cases have the following general form:

$$\frac{\partial X(z,t)}{\partial t} = -\frac{\partial F(X(z,t))}{\partial z} + D_0 \frac{\partial^2 X(z,t)}{\partial z^2}. \tag{1}$$

Here $X(z,t)$ is the space- and time- dependent concentration of suspended solids. $F(X(z,t))$ is the total convective flux, which is different for the two test cases, and will be discussed further below.

The required DAE for each test case is obtained from the PDE above by discretizing all the functions of z, and the partial derivatives w.r.t z, but retaining the continuous forms of the time derivative and functions of time. Thus the spatial derivatives are replaced by algebraic expressions, and the PDE therefore becomes an ordinary differential equation in time. We implement the spatial discretization using the method of orthogonal collocation on finite elements [3, 4, 5, 6]. We follow the treatment in [6] for the discretization and collocation procedure.

2 The Orthogonal Collocation Method

In this section we give a brief summary of the salient features of the orthogonal collocation method. A detailed description can be found in [3, 6]. This method is one of the *weighted residual methods* used to solve PDEs. Consider a function $\phi(z,t)$ defined over a certain spatial domain Ω, which depends on the two independent variables (z,t). Let the space- and- time- evolution of $\phi(z,t)$ be governed by a PDE :

$$\mathcal{D}\,\phi(z,t) = 0, \tag{2}$$

where $\mathcal{D}$ is a differential operator. The PDE is supplemented by boundary conditions for $\phi(z,t)$ on the boundary of the domain Ω, and initial conditions giving the value of $\phi(z,t)$ at time $t = 0$.

In a weighted residual method, we seek an approximate solution $\tilde{\phi}(z,t)$ of Eq.(2), which can be expressed as a sum of known polynomial functions depending only on z, with unknown coefficients depending only on t:

$$\tilde{\phi}(z,t) = \sum_{k=0}^{n} a_k(t)\,\theta_k(z). \tag{3}$$

The functions $\{\theta_k(z)\}$ are known, and the coefficients $\{a_k(t)\}$ have to be determined so that the solution satisfies the PDE and the boundary and initial conditions in an ‘optimal’ sense [3].

We first form the *residual* of $\mathcal{D}$, $R_n(z,t)$. It is given by:

$$R_n(z,t) = \mathcal{D}\,\tilde{\phi}(z,t). \tag{4}$$

$R_n(z,t)$ will be a continuous function of z and t. The approximate solution is then found by demanding that the *average* value of $R_n(z,t)$ (over the domain Ω) should be zero. We perform this average using some weighting function $W(z)$. That is:

$$\int_{\Omega} W(z)\, R_n(z,t)\, dz = 0. \tag{5}$$

We can evaluate the average instead by using a discrete set of m points:

$$\sum_{i=1}^{m} W(z_i)\, R_n(z_i,t) = 0. \tag{6}$$

Now in the *collocation method*, we simply choose the weights $\{W(z_i)\}$ to be Dirac delta functions at a particular set of points $\{z_j\}$, $j = 1..m$, called *collocation points*. From Eq.(6) above we have:

$$\begin{aligned} \textstyle\sum_i^m \delta(z_i - z_j)\, R_n(z_i,t) &= 0, \quad j = 1, \ldots, m; \\ \Rightarrow R_n(z_j,t) &= 0, \quad j = 1, \ldots, m. \end{aligned} \tag{7}$$

In the *orthogonal collocation method*, which is usually employed, the collocation points $\{z_j\}$ are chosen as the roots (zeroes) of one member of a set of orthogonal polynomials, usually the *Jacobi polynomials* [7]. Let the domain of interest be given by the interval $[z_0, z_{n+1}]$. Using the n zeroes of a Jacobi polynomial $G_n(\alpha+1, \beta+1, z)$ located in $[z_0, z_{n+1}]$, together with the two end-points of the domain - z_0 and z_{n+1}, the approximate solution is constructed using *Lagrange interpolation* [7]. (See further sections below for notes on Jacobi polynomials and Lagrange interpolation.) That is,

$$\tilde{\phi}(z,t) = \sum_{k=0}^{n} \phi(z_k,t)\, \ell_k(z)\, . \tag{8}$$

Comparing Eqs.(3) and (8) above, we note that the unknown coefficients $\{a_k(t)\}$ are just the values of the solution ϕ evaluated at the collocation points (the zeroes of the Jacobi polynomial and the end-points), ($\{\phi(z_k,t)\}$, $k = 0, \ldots, n+1$), and the polynomials $\{\theta_k(z)\}$ are just *Lagrange polynomials*.

A weighted residual method such as the orthogonal collocation method described above can be applied over the entire spatial domain Ω, and increased accuracy can be obtained by increasing the order n of the polynomials used. However, a better strategy is to use a *finite element* method. In such a method, the domain of interest is first divided into many smaller sub-domains or ‘elements’. Then a weighted residual method is applied within each element. Usually low-order approximations of the residuals are sufficient. Additional constraints are imposed by demanding the continuity of the approximate solution, and one or more of its derivatives, (or that of other quantities), at the boundaries between elements [3].

2.1 Lagrange Interpolation

For simplicity, we shall consider Lagrange interpolation in one dimension [3]. The method can be easily extended to multiple dimensions. Consider a set of points $\{x_0, x_1, x_2, \ldots, x_n\}$ located on the X axis. Suppose data corresponding to a certain quantity f are provided at these points; that is, we know the values $\{f(x_i)\}$ at these $n+1$ points. Using these values, we must find an approximation for the function $f(x)$ over the interval $[x_0, x_n]$. The simplest thing to do is to approximate $f(x)$ by a polynomial curve passing through the values $\{f(x_i)\}$. This can be done easily using the *Lagrange interpolation formula* to construct the interpolating polynomial using the $\{x_i\}$ as ‘nodes’. We thus have:

$$f(x) \simeq \sum_{i=0}^{n} \ell_i(x)\, f(x_i). \tag{9}$$

Here $\{\ell_i(x)\}$ are the *Lagrange polynomials*, of degree n (since we know $(n+1)$ constants, we can determine a polynomial of degree n). These polynomials are orthonormal. That is,

$$\ell_i(x_j) = \delta_{ij}\ . \tag{10}$$

As an example, we shall find the interpolating polynomial $f(x)$, given the two nodes $\{x_0, x_1\}$, and the values of $f(x)$ at these points. In this case, $f(x)$ will be a straight line connecting the two points. Using the interpolation formula (Eq.(9)), we have:

$$f(x) = \ell_0(x)\, f(x_0) + \ell_1(x)\, f(x_1). \tag{11}$$

For any x located between x_0 and x_1, we can use the property of a straight line that it has constant slope:

$$\frac{f(x_1) - f(x)}{(x_1 - x)} = \frac{f(x_1) - f(x_0)}{(x_1 - x_0)}. \tag{12}$$

Rearranging terms gives us the Lagrange interpolation formula:

$$f(x) = \frac{(x - x_1)}{(x_0 - x_1)}\, f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)}\, f(x_1). \tag{13}$$

From the above equation, we see that the Lagrange polynomials are given by:

$$\begin{aligned} \ell_0(x) &= \frac{(x - x_1)}{(x_0 - x_1)} \\ \ell_1(x) &= \frac{(x - x_0)}{(x_1 - x_0)} \end{aligned} \tag{14}$$

It can be verified that these are orthonormal.

Extending the discussion above to $(n+1)$ points, we can write a general expression for the Lagrange polynomials as follows:

$$\ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}. \tag{15}$$

We can rewrite $\ell_i(x)$ in a different form by first defining a polynomial $p(x)$ as:

$$\begin{aligned} p(x) &= \prod_{j=0}^{n} (x - x_j); \\ p^{(1)}(x_j) &= \left.\frac{dp}{dx}\right|_{x=x_j}. \end{aligned} \tag{16}$$

Therefore,

$$\ell_i(x) = \frac{p(x)}{(x - x_i)\, p^{(1)}(x_j)}. \tag{17}$$

By rearranging Eq.(17) and after some algebra, we can obtain explicit expressions for the first and second derivatives $\ell_i^{(1)}(x)$ and $\ell_i^{(2)}(x)$ [4], evaluated at a particular point $x = x_j$, in terms of $p(x)$ and its derivatives. There are two cases to consider: $i = j$, and $i \neq j$. We thus have [4]:

1. $i = j$:

We obtain a general expression for the m-th derivative of $\ell_i(x)$, $\ell_i^{(m)}(x)$ (evaluated at x_j) only in terms of $p(x)$ and its derivatives, when $i = j$:

$$\ell_i^{(m)}(x_i) = \frac{1}{m+1} \frac{p^{(m+1)}(x_i)}{p^{(1)}(x_i)} . \tag{18}$$

The first and second derivatives are therefore given by:

$$\begin{aligned} \ell_i^{(1)}(x_i) &= \frac{1}{2} \frac{p^{(2)}(x_i)}{p^{(1)}(x_i)} ; \\ \ell_i^{(2)}(x_i) &= \frac{1}{3} \frac{p^{(3)}(x_i)}{p^{(1)}(x_i)} . \end{aligned} \tag{19}$$

2. $i \neq j$:

In this case, it is not possible to obtain a general expression for $\ell_i^{(m)}(x)$ in terms of only $p(x)$ and its derivatives. We arrive at the following expressions for the first and second derivatives:

$$\ell_i^{(1)}(x_j) = \frac{1}{(x_j - x_i)} \frac{p^{(1)}(x_j)}{p^{(1)}(x_i)} ; \tag{20}$$

and

$$\begin{aligned} \ell_i^{(2)}(x_j) &= \frac{1}{(x_j - x_i)} \left(\frac{p^{(2)}(x_j)}{p^{(1)}(x_i)} - 2\, \ell_i^{(1)}(x_j) \right) \\ &= 2\, \ell_i^{(1)}(x_j) \left(\ell_i^{(1)}(x_i) - \frac{1}{(x_j - x_i)} \right) . \end{aligned} \tag{21}$$

2.2 Jacobi Polynomials

There are two kinds of Jacobi polynomials [7], $P_n(\alpha, \beta, x)$ and $G_n(\alpha+\beta+1, \beta+1, x)$, where ($\alpha$, $\beta > -1$). The polynomials $P_n(\alpha, \beta, x)$ form a complete orthogonal system in the interval $[-1, 1]$, while $G_n(\alpha+\beta+1, \beta+1, x)$ are orthogonal over $[0, 1]$. We shall be concerned only with the latter. They are defined by:

$$G_n(\alpha+\beta+1, \beta+1, x) = \frac{\Gamma(\beta+1+n)}{\Gamma(\alpha+\beta+1+2n)} \sum_{m=0}^{n} (-1)^m \left(\begin{array}{c} n \\ m \end{array} \right) \frac{\Gamma(\alpha+\beta+1+2n-m)}{\Gamma(\beta+1+n-m)}\, x^{n-m} . \tag{22}$$

They are orthogonal w.r.t the weight function:

$$w(x) = (1-x)^{\alpha}\, x^{\beta} . \tag{23}$$

That is,

$$\int_0^1 w(x)\, G_n(\alpha+\beta+1, \beta+1, x)\, G_m(\alpha+\beta+1, \beta+1, x)\; dx = C_n\, \delta_{nm} . \tag{24}$$

The normalization constant C_n is given by:

$$C_n = \frac{n!\, \Gamma(n+\beta+1)\, \Gamma(n+\alpha+1)\, \Gamma(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)\, \Gamma^2(2n+\alpha+\beta+1)} . \tag{25}$$

For a given pair (α, β), let us write

$$G_n(\alpha+\beta+1, \beta+1, x) \equiv G_n(x)\,. \qquad (26)$$

The $\{G_n(x)\}$ satisfy the recurrence relation:

$$G_{n+1}(x) = (x - a_n)\, G_n(x) - b_n\, G_{n-1}(x)\,, \qquad (27)$$

for $n = 0, 1, 2\ldots$. The coefficients are given by:

$$\begin{aligned} a_n &= \frac{2n\,(n+\alpha+\beta+1) + (\beta+1)\,(\alpha+\beta)}{(2n+\alpha+\beta)\,(2n+\alpha+\beta+2)} \\ b_n &= \frac{n\,(n+\alpha)\,(n+\beta)\,(n+\alpha+\beta)}{(2n+\alpha+\beta-1)\,(2n+\alpha+\beta)^2\,(2n+\alpha+\beta+1)}\,. \end{aligned} \qquad (28)$$

Also, $G_0(x) = 1$, and by definition, $G_{-1}(x) = 0$. We can compute other polynomials for higher values of n by simply using the recurrence relation successively. The values of α and β determine the location of the roots of the Jacobi polynomial within the interval $[0, 1]$ [5, 8]. Setting $(\alpha = \beta = 0)$ is the most common choice.

2.3 Zeroes of Jacobi Polynomials

In order to implement the collocation procedure, we have to find the n zeroes of a Jacobi polynomial $G_n(x)$ numerically. We proceed in the following way. We first write out the recurrence relation in Eq.(27) explicitly for the first few values of n:

$$\begin{aligned} G_1(x) &= (x-a_0)\, G_0(x) - b_0\, G_{-1}(x) \\ &= (x-a_0).1\; - 0 \\ &= (x-a_0)\,; \\[1em] G_2(x) &= (x-a_1)\, G_1(x) - b_1\, G_0(x) \\ &= (x-a_1)\,(x-a_0)\, G_0(x) - b_1\, G_0(x) \\ &= (x-a_1)\,(x-a_0).1 - b_1.1 \\ &= (x-a_1)\,(x-a_0)\,; \\[1em] G_3(x) &= (x-a_2)\, G_2(x) - b_2\, G_1(x) \\ &= (x-a_2)\,[\,(x-a_1)\,(x-a_0)\, G_0(x) - b_1\, G_0(x)\,] - b_2\,(x-a_0) \\ &= (x-a_2)\,[\,(x-a_1)\,(x-a_0) - b_1\,] - b_2\,(x-a_0)\,, \end{aligned} \qquad (29)$$

and so on for $n = 4, 5, \ldots$. From the above expressions, we notice that the polynomials $G_n(x)$ can be written as the *determinants* of corresponding square matrices of order n which have the form:

$$\begin{aligned} G_1(x) &= det\,[\,(x-a_0)\,]\,; \\[1em] G_2(x) &= det \begin{bmatrix} (x-a_0) & -\sqrt{b_1} \\ -\sqrt{b_1} & (x-a_1) \end{bmatrix}; \\[1em] G_3(x) &= det \begin{bmatrix} (x-a_0) & -\sqrt{b_1} & 0 \\ -\sqrt{b_1} & (x-a_1) & -\sqrt{b_2} \\ 0 & -\sqrt{b_2} & (x-a_2) \end{bmatrix}. \end{aligned} \qquad (30)$$

Finding the zeroes of $\{G_1(x), G_2(x), G_3(x), \ldots\}$, is just equivalent to setting the determinants above to zero. However, notice that doing this yields the characteristic (or eigenvalue) equations for the symmetric tridiagonal matrices whose diagonals have the coefficients $\{a_i\}$ and the subdiagonals are made up of the coefficients $\{\sqrt{b_i}\}$. That is, for a given n, the zeroes of $G_n(x)$ are given by the eigenvalues of a symmetric tridiagonal matrix of dimension $[\,n \times n\,]$, whose diagonal is the n - dimensional vector $Diag$:

$$Diag = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1} \end{bmatrix}, \tag{31}$$

and the subdiagonals are given by the $(n-1)$ - dimensional vector Sub:

$$Sub = \begin{bmatrix} \sqrt{b_1} \\ \sqrt{b_2} \\ \vdots \\ \sqrt{b_{n-1}} \end{bmatrix}. \tag{32}$$

3 The PDE for continuous sedimentation

For continuous sedimentation, the PDE, Eq.(1), is given by:

$$\frac{\partial X(z,t)}{\partial t} = -\frac{\partial F(X(z,t))}{\partial z} + D_0\, \frac{\partial^2 X(z,t)}{\partial z^2}. \tag{33}$$

where the convective flux F is given by the sum of the gravitational settling and the bulk flow. We now write F in a form different from that presented in [2]. In [2], the source flux flowing into the clarifier at the location of the inlet was modelled by a Dirac delta function. It turns out that this is not the right thing to do. Instead, we now write the flux in the following form:

$$\begin{aligned} F(X(z,t),z,t) \;&=\; G(X(z,t)) \\ &\quad + X(z,t)\,\left[\frac{Q_u(t)}{A}\,\theta(z-z_f) - \frac{Q_e(t)}{A}\,\theta(z_f-z)\right] \\ &\quad + X_f(t)\,\frac{Q_f(t)}{A}\,\theta(z-z_f)\,. \end{aligned} \tag{34}$$

Here, $G(X(z,t))$ is the gravitational settling flux, and is given by

$$G(X(z,t)) = X(z,t)\, v_s(X(z,t)), \tag{35}$$

where $v_s(X(z,t))$ is the Vesilind settling velocity function having the exponential form

$$v_s(X(z,t)) = v_o e^{-n\,X(z,t)}, \tag{36}$$

with v_o and n being constant parameters [1]. Also, in (34), $Q_e(t)/A$ is defined as the upward bulk velocity (the effluent), and $Q_u(t)/A$ the downward bulk velocity (the underflow). A is the area of cross section of the clarifier tank. Notice that writing the flux in this form means that we are now using a simple picture wherein there is a net flow of liquid downwards below the inlet, which is a sum of the underflow and source fluxes, and a net flow upward above the inlet, consisting of the effluent.

The *Heaviside theta function*, or the *unit step function*, is defined as follows:

$$\theta(z) = \begin{cases} 0, & z < 0 \\ 1, & z \geq 0 \end{cases}. \tag{37}$$

Its derivative is given by the Dirac delta function:

$$\theta'(z) \equiv \frac{d\theta(z)}{dz} = \delta(z) \,. \tag{38}$$

$\theta(z)$ also has the property:

$$\theta(z) = 1 - \theta(-z) \,. \tag{39}$$

We shall use these properties later when we transform the PDE to a DAE.

3.1 Initial and Boundary conditions

As the initial condition for the concentration, we assume a given concentration profile. As a particular example, we first take the simplest case of a constant concentration profile:

$$\begin{aligned} X(z, t = 0) &= X_0(z) \\ &= X_0, \end{aligned} \tag{40}$$

where X_0 is a constant for all z.

From the discussion in [2], we are led to the following boundary conditions for the clarifier:

$$\begin{aligned} \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=0} &= 0 \\ \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=L} &= 0. \end{aligned} \tag{41}$$

4 The PDE for batch sedimentation

For the batch sedimentation case, the convective flux comprises only the gravitational settling, since there are no source or bulk flows present. That is, $F(X(z,t)) \equiv G(X(z,t))$. Therefore, the PDE simply becomes:

$$\frac{\partial X(z,t)}{\partial t} = -\frac{\partial G(X(z,t))}{\partial z} + D_0 \frac{\partial^2 X(z,t)}{\partial z^2}. \tag{42}$$

4.1 Initial and Boundary conditions

We use the same initial condition as that for the continuous sedimentation case. That is,

$$\begin{aligned} X(z, t = 0) &= X_0(z) \\ &= X_0 \,. \end{aligned} \tag{43}$$

We have derived the following boundary conditions for the batch sedimentation case in [2]:

$$\begin{aligned} G(X(0,t)) - D_0 \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=0} &= 0 \\ G(X(L,t)) - D_0 \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=L} &= 0. \end{aligned} \tag{44}$$

5 Discretization of the PDE

We will first set up the discretization and collocation points [6, 8] for the general form of the PDE given in Eq.(1), and then apply the procedure for the two test case conditions separately.

We first use a normalized dimensionless variable h to replace the z- coordinate in the PDE of Eq.(1), defined by:

$$h = z/L, \tag{45}$$

so that as z varies over $[0, L]$, h correspondingly varies over $[0, 1]$.

Therefore Eq.(1) becomes:

$$\frac{\partial X(L\,h,t)}{\partial t} = -\frac{1}{L}\frac{\partial F(X(L\,h,t))}{\partial h} + \frac{D_0}{L^2}\frac{\partial^2 X(L\,h,t)}{\partial h^2}. \tag{46}$$

We divide the domain [0,1] into N_E elements or intervals, by defining $(N_E + 1)$ nodes: $\{H_1 \equiv 0, H_2, H_3, \ldots, H_{N_E+1} \equiv 1\}$. The width of the i-th element is thus given by:

$$\Delta_i = H_{i+1} - H_i, \quad i = 1, \ldots, N_E. \tag{47}$$

We now need to define a further internal ‘reduced’ variable on each element, such that every element is again rescaled to $[0, 1]$. Thus for the i-th element $(i = 1, \ldots N_E)$, we define this reduced variable $\xi^{(i)}$ as follows:

$$\xi^{(i)} = \frac{h - H_i}{\Delta_i}, \tag{48}$$

so that $\xi^{(i)}$ varies over $[0, 1]$ as h varies over $[H_i, H_{i+1}]$.

We use the values of the quantity X at the end-points of every interval i, and those at $N(i)$ *interior collocation points*, to approximate X over this interval using the Lagrange interpolation formula as in Eq.(9). These interior collocation points are chosen as the zeroes of orthogonal Jacobi polynomials, as discussed above. We thus have a total of $(N(i)+2)$ coefficients, obtained by evaluating the concentration X at the $N(i) + 2$ points $\{\xi_0^{(i)} \equiv 0, \xi_1^{(i)}, \ldots, \xi_{N(i)}^{(i)}, \xi_{N(i)+1}^{(i)} \equiv 1\}$, which can determine the polynomial approximation $X^{(i)}$ of X over this interval (of degree $N(i) + 1$). We first write:

$$X^{(i)}(L\,h,t) = X^{(i)}(\,L\,(\xi^{(i)}\Delta_i + H_i), t\,) = X^{(i)}(\xi^{(i)}, t) \tag{49}$$

$X^{(i)}(\xi^{(i)}, t)$ is thus given by:

$$X^{(i)}(\xi^{(i)}, t) \simeq \sum_{k=0}^{N(i)+1} \ell_k^{(i)}(\xi^{(i)})\; X^{(i)}(\xi_k^{(i)}, t). \tag{50}$$

Here the $\{\ell_k^{(i)}(\xi^{(i)})\}$ are Lagrange polynomials of degree $(N(i) + 1)$. The total number of unknowns, $\{X^{(i)}(\xi_k^{(i)}, t)\}$, is therefore equal to the total number of collocation points, N_T, which is the sum (over all intervals) of all the collocation points in every interval - including the interior ones and the end-points of the interval. That is,

$$N_T = \sum_{i=1}^{N_E} (\,N(i) + 2\,)\,. \tag{51}$$

The total number of interior collocation points, N_C, is given by:

$$N_C = \sum_{i=1}^{N_E} N(i)\,. \tag{52}$$

Therefore we have:

$$N_T = N_C + 2\,N_E\,. \tag{53}$$

In order to determine the N_T unknowns uniquely, we need at least N_T equations in the unknowns. We can account for these as follows: there will be N_C DAEs resulting from the discretization of the PDE at the N_C interior collocation points. In addition, there are two equations in the two collocation points at the domain boundaries ($z = 0, L$), given by the boundary conditions in Eq.(44). Also, there are two equations arising from the continuity of the concentration $X(z,t)$ and its first derivative $\partial X/\partial z$, at each of the $(N_E - 1)$ nodes $\{H_2, \ldots, H_{N_E}\}$. Thus the total number of equations we have at our disposal is $N_C + 2 + 2\,(N_E - 1) \equiv N_T$. In addition, there are N_C initial conditions available for solving the DAE at the N_C interior collocation points.

Using the expansion (50), we can define the derivatives of X as well. Thus,

$$\left.\frac{\partial X^{(i)}(\xi^{(i)},t)}{\partial \xi^{(i)}}\right|_{\xi^{(i)}=\xi_j^{(i)}} = \sum_{k=0}^{N(i)+1} \left.\frac{\partial \ell_k^{(i)}(\xi^{(i)})}{\partial \xi^{(i)}}\right|_{\xi^{(i)}=\xi_j^{(i)}} X^{(i)}(\xi_k^{(i)},t). \tag{54}$$

Similarly,

$$\left.\frac{\partial^2 X^{(i)}(\xi^{(i)},t)}{\partial {\xi^{(i)}}^2}\right|_{\xi^{(i)}=\xi_j^{(i)}} = \sum_{k=0}^{N(i)+1} \left.\frac{\partial^2 \ell_k^{(i)}(\xi^{(i)})}{\partial {\xi^{(i)}}^2}\right|_{\xi^{(i)}=\xi_j^{(i)}} X^{(i)}(\xi_k^{(i)},t). \tag{55}$$

We set

$$\begin{aligned}
X^{(i)}(\xi_j^{(i)},t) &= X_j^{(i)}(t)\,; \\
\left.\frac{\partial \ell_k^{(i)}(\xi^{(i)})}{\partial \xi^{(i)}}\right|_{\xi^{(i)}=\xi_j^{(i)}} &= A_{j,k}^{(i)}\,; \\
\left.\frac{\partial^2 \ell_k^{(i)}(\xi^{(i)})}{\partial {\xi^{(i)}}^2}\right|_{\xi^{(i)}=\xi_j^{(i)}} &= B_{j,k}^{(i)}\,; \\
i &= 1, \ldots, N_E\,, \\
j &= 0, \ldots, N(i)+1\,, \\
k &= 0, \ldots, N(i)+1\,.
\end{aligned} \tag{56}$$

Therefore we can rewrite Eqns.(54) and (55) as:

$$\begin{aligned}
\left.\frac{\partial X^{(i)}(\xi^{(i)},t)}{\partial \xi^{(i)}}\right|_{\xi^{(i)}=\xi_j^{(i)}} &= \sum_{k=0}^{N(i)+1} A_{j,k}^{(i)}\, X_k^{(i)}(t) \\
\left.\frac{\partial^2 X^{(i)}(\xi^{(i)},t)}{\partial {\xi^{(i)}}^2}\right|_{\xi^{(i)}=\xi_j^{(i)}} &= \sum_{k=0}^{N(i)+1} B_{j,k}^{(i)}\, X_k^{(i)}(t)
\end{aligned} \tag{57}$$

Note that the square matrices $A^{(i)}$ and $B^{(i)}$ both have the dimensions $(N(i)+2) \times (N(i)+2)$.

Using the discretized version of the concentration and its derivatives as indicated above, we finally arrive at the required DAEs for the concentration X at each interior collocation point. These DAEs are supplemented by the discretized versions of the initial condition at the interior collocation points, the boundary conditions at the domain boundaries, and the continuity conditions for the concentration and its first derivative at the (interior) element boundaries. We now consider the two test cases separately.

6 The DAE for continuous sedimentation

We use the explicit form of the derivative of the flux F in Eq.(33). The derivative of the gravitational flux is given by:

$$\begin{aligned} \frac{\partial G(X(z,t))}{\partial z} &= (1 - n\,X(z,t))\; v_0\, e^{-n\,X(z,t)}\; \frac{\partial X(z,t)}{\partial z} \\ &= (1 - n\,X(z,t))\; \frac{G(X(z,t))}{X(z,t)}\; \frac{\partial X(z,t)}{\partial z}. \end{aligned} \tag{58}$$

We use the properties of $\theta(z)$ - Eqns.(38) and (39), to simplify the other terms appearing in the flux. We also use the relation [2]:

$$\frac{Q_f(t)}{A} = \frac{Q_u(t)}{A} + \frac{Q_e(t)}{A} \tag{59}$$

to eliminate $Q_e(t)/A$, since the effluent flux is an output of the calculation, and is not known beforehand.

After some algebra, we arrive at the following expression for the derivative of the flux :

$$\begin{aligned} \frac{\partial F(X(z,t))}{\partial z} &= \left[(1 - n\,X(z,t))\; v_0\; e^{-n\,X(z,t)} + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A}\,\theta(z_f - z) \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad + \;(X(z,t) + X_f(t))\; \frac{Q_f(t)}{A}\; \delta(z - z_f)\,. \end{aligned} \tag{60}$$

Therefore the PDE for continuous sedimentation becomes:

$$\begin{aligned} \frac{\partial X(z,t)}{\partial t} &= -\left[(1 - n\,X(z,t))\; v_0\; e^{-n\,X(z,t)} + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A}\,\theta(z_f - z) \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad - (X(z,t) + X_f(t))\; \frac{Q_f(t)}{A}\; \delta(z - z_f) \\ &\quad + D_0\, \frac{\partial^2 X(z,t)}{\partial z^2}\,. \end{aligned} \tag{61}$$

For the convenient numerical implementation of the above PDE as a DAE, we use the defining numerical values of $\theta(z - z_f)$. We shall also represent the Dirac delta function by a rectangular pulse of unit height and width $2\,\sigma$, centred at $z = z_f$. σ is assumed to be small.

Therefore the PDE in Eq.(61) will consist of three parts:

1. for $\{\,0 \le z \le z_f - \sigma\,\}$:

$$\begin{aligned} \frac{\partial X(z,t)}{\partial t} &= -\left[(1 - n\,X(z,t))\; v_0\; e^{-n\,X(z,t)} + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A} \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad + D_0\, \frac{\partial^2 X(z,t)}{\partial z^2}\,; \end{aligned} \tag{62}$$

2. for $\{ z_f - \sigma < z < z_f + \sigma \}$:

$$\begin{aligned} \frac{\partial X(z,t)}{\partial t} &= - \left[(1 - n\, X(z,t))\ v_0\ e^{-n\, X(z,t)} + \frac{Q_u(t)}{A} \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad - (\, X(z,t) \,+\, X_f(t)\,)\ \frac{Q_f(t)}{A} \\ &\quad + D_0\, \frac{\partial^2 X(z,t)}{\partial z^2}\, ; \end{aligned} \tag{63}$$

3. for $\{ z_f + \sigma \le z \le L \}$:

$$\begin{aligned} \frac{\partial X(z,t)}{\partial t} &= - \left[(1 - n\, X(z,t))\ v_0\ e^{-n\, X(z,t)} + \frac{Q_u(t)}{A} \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad + D_0\, \frac{\partial^2 X(z,t)}{\partial z^2}\, . \end{aligned} \tag{64}$$

Using Eqns.(50)-(57), we can now write the DAE for continuous sedimentation. Let us specify the finite elements such that the unit pulse (representing the delta function) spans element N_D. Therefore, the N_D-th element is of width $2\,\sigma$. The DAE is written for all the N_C interior collocation points. Again, the DAE will be written in three parts:

1. for $\{ t = 0\,;\ i = 1, \ldots\ N_D - 1\,;\ j = 1, \ldots\ N(i) \}$

$$\begin{aligned} \frac{dX_j^{(i)}(t)}{dt} &= -\frac{1}{L\Delta_i} \left[\left(1 - n\, X_j^{(i)}(t)\right)\ v_0\ e^{-n\, X_j^{(i)}(t)} + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A} \right] \sum_{k=0}^{N(i)+1} A_{j,k}^{(i)}\, X_k^{(i)}(t) \\ &\quad + \frac{D_0}{L^2\Delta_i^2} \sum_{k=0}^{N(i)+1} B_{j,k}^{(i)}\, X_k^{(i)}(t)\, ; \end{aligned} \tag{65}$$

We can group the summands on the RHS of the above equation to obtain:

$$\frac{dX_j^{(i)}(t)}{dt} = \sum_{k=0}^{N(i)+1} \left(-\frac{1}{L\Delta_i} \left[\left(1 - n\, X_j^{(i)}(t)\right)\ v_0\ e^{-n\, X_j^{(i)}(t)} + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A} \right] A_{j,k}^{(i)} + \frac{D_0}{L^2\Delta_i^2}\, B_{j,k}^{(i)} \right) X_k^{(i)}(t)\, . \tag{66}$$

Similarly, we have:

2. for $\{ t = 0\,;\ i = N_D\,;\ j = 1, \ldots\ N(N_D) \}$

$$\begin{aligned} \frac{dX_j^{(i)}(t)}{dt} &= \sum_{k=0}^{N(i)+1} \left(-\frac{1}{L\Delta_i} \left[\left(1 - n\, X_j^{(i)}(t)\right)\ v_0\ e^{-n\, X_j^{(i)}(t)} + \frac{Q_u(t)}{A} \right] A_{j,k}^{(i)} + \frac{D_0}{L^2\Delta_i^2}\, B_{j,k}^{(i)} \right) X_k^{(i)}(t) \\ &\quad - \left(X_j^{(i)}(t) \,+\, X_f(t) \right) \frac{Q_f(t)}{A}\, . \end{aligned} \tag{67}$$

3. for $\{ t = 0\,;\ i = N_D + 1, \ldots\ N_E\,;\ j = 1, \ldots\ N(i) \}$

$$\frac{dX_j^{(i)}(t)}{dt} = \sum_{k=0}^{N(i)+1} \left(-\frac{1}{L\Delta_i} \left[\left(1 - n\, X_j^{(i)}(t)\right)\ v_0\ e^{-n\, X_j^{(i)}(t)} + \frac{Q_u(t)}{A} \right] A_{j,k}^{(i)} + \frac{D_0}{L^2\Delta_i^2}\, B_{j,k}^{(i)} \right) X_k^{(i)}(t)\, . \tag{68}$$

The initial condition, Eq.(40), is implemented as follows, again for the N_C interior collocation points:

$$
\begin{aligned}
X_j^{(i)}(t=0) &= X_{j0}^{(i)} = X_0 ; \\
i &= 1,\ldots,N_E ; \\
j &= 1,\ldots,N(i) .
\end{aligned}
\tag{69}
$$

The two boundary conditions, Eqns.(41), are implemented at the collocation points corresponding to $z=0$ and $z=L$:

$$
\begin{aligned}
\frac{D_0}{L\,\Delta_1}\sum_{k=0}^{N(1)+1} A_{0,k}^{(1)}\,X_k^{(1)}(t) &= 0 ; \\
\frac{D_0}{L\,\Delta_{N_E}}\sum_{k=0}^{N(N_E)+1} A_{N(N_E)+1,k}^{(N_E)}\,X_k^{(N_E)}(t) &= 0 .
\end{aligned}
\tag{70}
$$

We now have to implement the element boundary conditions. As discussed earlier, we assume that both the concentration X and its first derivative $\partial X/\partial z$ are continuous at all the interior nodes which are the boundaries between neighbouring elements. This is implemented as follows: for ($i=1,\ldots,N_E-1$),

$$
\begin{aligned}
X_0^{(i+1)}(t) &= X_{N(i)+1}^{(i)}(t); \\
\frac{1}{L\,\Delta_{i+1}}\sum_{k=0}^{N(i+1)+1} A_{0,k}^{(i+1)}\,X_k^{(i+1)}(t) &= \frac{1}{L\,\Delta_i}\sum_{k=0}^{N(i)+1} A_{N(i)+1,k}^{(i)}\,X_k^{(i)}(t).
\end{aligned}
\tag{71}
$$

7 The DAE for batch sedimentation

Using the explicit form of ($\partial G/\partial z$) derived in Eq.(58), the PDE for batch sedimentation has the form:

$$
\frac{\partial X(z,t)}{\partial t} = -\left((1-n\,X(z,t))\,v_0\,e^{-n\,X(z,t)}\right)\frac{\partial X(z,t)}{\partial z} + D_0\,\frac{\partial^2 X(z,t)}{\partial z^2}. \tag{72}
$$

Using Eqns.(50)-(57), we write the DAE for batch sedimentation just as we did for the continuous case in the previous section. Again, the DAE is written for all the N_C interior collocation points.

$$
\frac{dX_j^{(i)}(t)}{dt} = -\frac{1}{L\Delta_i}\left(\left(1-n\,X_j^{(i)}(t)\right)\,v_0\,e^{-n\,X_j^{(i)}(t)}\right)\sum_{k=0}^{N(i)+1} A_{j,k}^{(i)}\,X_k^{(i)}(t)+\frac{D_0}{L^2\Delta_i^2}\sum_{k=0}^{N(i)+1} B_{j,k}^{(i)}\,X_k^{(i)}(t), \tag{73}
$$

for:

$$
\begin{aligned}
t &> 0; \\
i &= 1,\ldots,N_E; \\
j &= 1,\ldots,N(i).
\end{aligned}
\tag{74}
$$

We can group the summands on the RHS of Eq.(73) as before, to obtain, finally:

$$
\frac{dX_j^{(i)}(t)}{dt} = \sum_{k=0}^{N(i)+1}\left[-\frac{1}{L\Delta_i}\left(\left(1-n\,X_j^{(i)}(t)\right)\,v_0\,e^{-n\,X_j^{(i)}(t)}\right)A_{j,k}^{(i)} + \frac{D_0}{L^2\Delta_i^2}\,B_{j,k}^{(i)}\right]X_k^{(i)}(t). \tag{75}
$$

The initial condition for the batch case, Eq.(43), is implemented as follows, again for the N_C interior collocation points:

$$\begin{aligned} X_j^{(i)}(t=0) &= X_{j0}^{(i)} = X_0\,; \\ i &= 1,\dots,N_E\,; \\ j &= 1,\dots,N(i)\,. \end{aligned} \tag{76}$$

The two corresponding boundary conditions for the batch case, Eqns.(44), are again implemented at the collocation points corresponding to $z=0$ and $z=L$:

$$\begin{aligned} \frac{D_0}{L\,\Delta_1}\sum_{k=0}^{N(1)+1} A_{0,k}^{(1)}\,X_k^{(1)}(t) &= G(X_0^{(1)}(t)) \\ &= X_0^{(1)}(t)\,v_0\,e^{-n\,X_0^{(1)}(t)}\,; \\ \frac{D_0}{L\,\Delta_{N_E}}\sum_{k=0}^{N(N_E)+1} A_{N(N_E)+1,k}^{(N_E)}\,X_k^{(N_E)}(t) &= G(X_{N(N_E)+1}^{(N_E)}(t)) \\ &= X_{N(N_E)+1}^{(N_E)}(t)\,v_0\,e^{-n\,X_{N(N_E)+1}^{(N_E)}(t)}\,. \end{aligned} \tag{77}$$

The element boundary conditions are implemented as follows, just as for the continuous case: for ($i = 1,\dots,N_E-1$),

$$\begin{aligned} X_0^{(i+1)}(t) &= X_{N(i)+1}^{(i)}(t); \\ \frac{1}{L\,\Delta_{i+1}}\sum_{k=0}^{N(i+1)+1} A_{0,k}^{(i+1)}\,X_k^{(i+1)}(t) &= \frac{1}{L\,\Delta_i}\sum_{k=0}^{N(i)+1} A_{N(i)+1,k}^{(i)}\,X_k^{(i)}(t). \end{aligned} \tag{78}$$

8 Examples

We shall first illustrate the conversion of the PDE for batch sedimentation, Eq.(42), to a DAE using the orthogonal collocation method on finite elements. Here we shall discuss the method in detail. Following this we present a brief illustration of the same method applied to the continuous sedimentation case.

8.1 An example for batch sedimentation

The PDE to be discretized is the following (using the dimensionless variable h):

$$\frac{\partial X(L\,h,t)}{\partial t} = -\frac{1}{L}\,\frac{\partial G(X(L\,h,t))}{\partial h} + \frac{D_0}{L^2}\,\frac{\partial^2 X(L\,h,t)}{\partial h^2}. \tag{79}$$

We divide the domain of interest $[0,1]$ into *two* elements, by defining three nodes $\{\,H_1 = 0, H_2 = 0.4, H_3 = 1\,\}$. On the first element, we locate one interior collocation point, and two on the second. We set $\alpha = \beta = 0$. Thus we have:

$$\begin{aligned}
\alpha &= 0\,;\\
\beta &= 0\,;\\
N_E &= 2\,;\\
i &= 1,\,2\\
\Delta_1 &= (H_2 - H_1) = 0.4\,;\\
\Delta_2 &= (H_3 - H_2) = 0.6\,;\\
N(1) &= 1\,;\\
N(2) &= 2\,;\\
N_C &= 3\,;\\
N_T &= 7\,;
\end{aligned} \tag{80}$$

Now the appropriate Jacobi polynomials are $(\,G_1(0,0,x),\; G_2(0,0,x)\,)$. These are given by:

$$\begin{aligned}
G_1(0,0,x) &= x - 1/2\,;\\
G_2(0,0,x) &= x^2 - x + 1/6\,;
\end{aligned} \tag{81}$$

Their roots are given by: (0.5), and $(0.21132,\ 0.78868)$ respectively. Thus the collocation points $\{\xi_j^{(i)}\}$ are given by:

$$\begin{aligned}
\xi_0^{(1)} &= 0.0\,;\\
\xi_1^{(1)} &= 0.5\,;\\
\xi_2^{(1)} &= 1.0\,;\\
\xi_0^{(2)} &= 0.0\,;\\
\xi_1^{(2)} &= 0.21132\,;\\
\xi_2^{(2)} &= 0.78868\,;\\
\xi_3^{(2)} &= 1.0\,;
\end{aligned} \tag{82}$$

The polynomial approximation to the concentration X over each element will then have the form in Eq.(50):

$$X^{(1)}(\xi^{(1)},t) = \sum_{k=0}^{2} \ell_k^{(1)}(\xi^{(1)})\; X^{(1)}(\xi_k^{(1)},t)\,;$$

$$X^{(2)}(\xi^{(2)},t) \quad = \quad \sum_{k=0}^{3} \ell_k^{(2)}(\xi^{(2)}) \; X^{(2)}(\xi_k^{(2)},t)\,. \tag{83}$$

The polynomials $\{p_i(x)\}$ of Eq.(16) used to define the required Lagrange polynomials and their derivatives over each interval are given by:

$$p_i(\xi^{(i)}) = \prod_{j=0}^{n} (\xi^{(i)} - \xi_j^{(i)}), \tag{84}$$

where $p_i(\xi^{(i)})$ indicates the polynomial on the i-th element. Thus we have:

$$\begin{aligned} p_1(\xi^{(1)}) &= (\xi^{(1)} - \xi_0^{(1)})\,(\xi^{(1)} - \xi_1^{(1)})\,(\xi^{(1)} - \xi_2^{(1)}) \\ &\equiv (\xi^{(1)} - 0.0)\,(\xi^{(1)} - 0.5)\,(\xi^{(1)} - 1.0)\,. \end{aligned} \tag{85}$$

and

$$\begin{aligned} p_2(\xi^{(2)}) &= (\xi^{(2)} - \xi_0^{(2)})\,(\xi^{(2)} - \xi_1^{(2)})\,(\xi^{(2)} - \xi_2^{(2)})\,(\xi^{(2)} - \xi_3^{(2)}) \\ &\equiv (\xi^{(2)} - 0.0)\,(\xi^{(2)} - 0.21132)\,(\xi^{(2)} - 0.78868)\,(\xi^{(2)} - 1.0)\,. \end{aligned} \tag{86}$$

From the above expressions for (p_1, p_2), the Lagrange polynomials, their derivatives, and hence the matrices $(A^{(1)}, B^{(1)})$ and $(A^{(2)}, B^{(2)})$ can be obtained, using Eqns.(17) - (19) and the definitions (56). We thus have [3, 4] (note that these matrices are the transposes of the ones in [3]):

$$A^{(1)} \equiv \begin{bmatrix} -3.0 & 4.0 & -1.0 \\ -1.0 & 0.0 & 1.0 \\ 1.0 & -4.0 & 3.0 \end{bmatrix} ; \tag{87}$$

$$B^{(1)} \equiv \begin{bmatrix} 4.0 & -8.0 & 4.0 \\ 4.0 & -8.0 & 4.0 \\ 4.0 & -8.0 & 4.0 \end{bmatrix} ; \tag{88}$$

$$A^{(2)} \equiv \begin{bmatrix} -7.00000 & 8.19615 & -2.19615 & 1.00000 \\ -2.73205 & 1.73205 & 1.73205 & -0.73205 \\ 0.73205 & -1.73205 & -1.73205 & 2.73205 \\ -1.00000 & 2.19615 & -8.19615 & 7.00000 \end{bmatrix} ; \tag{89}$$

$$B^{(2)} \equiv \begin{bmatrix} 24.00000 & -37.17691 & 25.17691 & -12.00000 \\ 16.39230 & -24.00000 & 12.00000 & -4.39230 \\ -4.39230 & 12.00000 & -24.00000 & 16.39230 \\ -12.00000 & 25.17691 & -37.17691 & 24.00000 \end{bmatrix} . \tag{90}$$

We can now write down explicitly the DAEs for the concentration at the $N_C = 3$ interior collocation points, Eq.(75). For the collocation point $\xi_1^{(1)}$ within the first element, we have:

$$\frac{dX_1^{(1)}(t)}{dt} = \sum_{k=0}^{2} \left[-\frac{1}{L\Delta_1} \left(\left(1 - n\,X_1^{(1)}(t) \right) \; v_0 \; e^{-n\,X_1^{(1)}(t)} \right) A_{1,k}^{(1)} + \frac{D_0}{L^2\Delta_1^2}\, B_{1,k}^{(1)} \right] X_k^{(1)}(t). \tag{91}$$

Expanding the sum above, we have:

$$\begin{aligned}
\frac{dX_1^{(1)}(t)}{dt} \;=\;& \left[-\frac{1}{L\Delta_1}\left(\left(1-n\,X_1^{(1)}(t)\right)\; v_0\; e^{-n\,X_1^{(1)}(t)}\right) A_{1,0}^{(1)} + \frac{D_0}{L^2\Delta_1^2}\,B_{1,0}^{(1)}\right] X_0^{(1)}(t) \\
&+\left[-\frac{1}{L\Delta_1}\left(\left(1-n\,X_1^{(1)}(t)\right)\; v_0\; e^{-n\,X_1^{(1)}(t)}\right) A_{1,1}^{(1)} + \frac{D_0}{L^2\Delta_1^2}\,B_{1,1}^{(1)}\right] X_1^{(1)}(t) \\
&+\left[-\frac{1}{L\Delta_1}\left(\left(1-n\,X_1^{(1)}(t)\right)\; v_0\; e^{-n\,X_1^{(1)}(t)}\right) A_{1,2}^{(1)} + \frac{D_0}{L^2\Delta_1^2}\,B_{1,2}^{(1)}\right] X_2^{(1)}(t)\,. \qquad (92)
\end{aligned}$$

Similarly at the two interior collocation points ($\xi_1^{(2)} = 0.21132$, $\xi_2^{(2)} = 0.78868$), we have the DAEs:

$$\begin{aligned}
\frac{dX_1^{(2)}(t)}{dt} &= \sum_{k=0}^{3}\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_1^{(2)}(t)\right)\; v_0\; e^{-n\,X_1^{(2)}(t)}\right) A_{1,k}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{1,k}^{(2)}\right] X_k^{(2)}(t)\,; \\
\frac{dX_2^{(2)}(t)}{dt} &= \sum_{k=0}^{3}\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_2^{(2)}(t)\right)\; v_0\; e^{-n\,X_2^{(2)}(t)}\right) A_{2,k}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{2,k}^{(2)}\right] X_k^{(2)}(t)\,. \qquad (93)
\end{aligned}$$

Expanding the sums again, we have:

$$\begin{aligned}
\frac{dX_1^{(2)}(t)}{dt} \;=\;& \left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_1^{(2)}(t)\right)\; v_0\; e^{-n\,X_1^{(2)}(t)}\right) A_{1,0}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{1,0}^{(2)}\right] X_0^{(2)}(t) \\
&+\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_1^{(2)}(t)\right)\; v_0\; e^{-n\,X_1^{(2)}(t)}\right) A_{1,1}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{1,1}^{(2)}\right] X_1^{(2)}(t) \\
&+\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_1^{(2)}(t)\right)\; v_0\; e^{-n\,X_1^{(2)}(t)}\right) A_{1,2}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{1,2}^{(2)}\right] X_2^{(2)}(t) \\
&+\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_1^{(2)}(t)\right)\; v_0\; e^{-n\,X_1^{(2)}(t)}\right) A_{1,3}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{1,3}^{(2)}\right] X_3^{(2)}(t)\,. \qquad (94)
\end{aligned}$$

and:

$$\begin{aligned}
\frac{dX_2^{(2)}(t)}{dt} \;=\;& \left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_2^{(2)}(t)\right)\; v_0\; e^{-n\,X_2^{(2)}(t)}\right) A_{2,0}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{2,0}^{(2)}\right] X_0^{(2)}(t) \\
&+\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_2^{(2)}(t)\right)\; v_0\; e^{-n\,X_2^{(2)}(t)}\right) A_{2,1}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{2,1}^{(2)}\right] X_1^{(2)}(t) \\
&+\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_2^{(2)}(t)\right)\; v_0\; e^{-n\,X_2^{(2)}(t)}\right) A_{2,2}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{2,2}^{(2)}\right] X_2^{(2)}(t) \\
&+\left[-\frac{1}{L\Delta_2}\left(\left(1-n\,X_2^{(2)}(t)\right)\; v_0\; e^{-n\,X_2^{(2)}(t)}\right) A_{2,3}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\,B_{2,3}^{(2)}\right] X_3^{(2)}(t)\,. \qquad (95)
\end{aligned}$$

The three DAEs above (Eqns.(92)-(95)) must be solved together with the initial conditions:

$$\begin{aligned}
X_1^{(1)}(t=0) &= X_{10}^{(1)} = X_0\,; \\
X_1^{(2)}(t=0) &= X_{10}^{(2)} = X_0\,; \\
X_2^{(2)}(t=0) &= X_{20}^{(2)} = X_0\,. \qquad (96)
\end{aligned}$$

The two boundary conditions (at $z = 0, L$) are now given by the equations:

$$\begin{aligned}
\frac{D_0}{L\,\Delta_1}\sum_{k=0}^{2} A^{(1)}_{0,k}\,X^{(1)}_k(t) &= G(X^{(1)}_0(t)) \\
&= X^{(1)}_0(t)\,v_0\,e^{-n\,X^{(1)}_0(t)}\,; \\
\frac{D_0}{L\,\Delta_2}\sum_{k=0}^{3} A^{(2)}_{3,k}\,X^{(2)}_k(t) &= G(X^{(2)}_3(t)) \\
&= X^{(2)}_3(t)\,v_0\,e^{-n\,X^{(2)}_3(t)}\,.
\end{aligned} \tag{97}$$

Expanding them, we have:

$$\begin{aligned}
\frac{D_0}{L\,\Delta_1}\Big(A^{(1)}_{0,0}\,X^{(1)}_0(t)+A^{(1)}_{0,1}\,X^{(1)}_1(t)+A^{(1)}_{0,2}\,X^{(1)}_2(t)\Big) &= G(X^{(1)}_0(t)) \\
&= X^{(1)}_0(t)\,v_0\,e^{-n\,X^{(1)}_0(t)}\,; \\
\frac{D_0}{L\,\Delta_2}\Big(A^{(2)}_{3,0}\,X^{(2)}_0(t)+A^{(2)}_{3,1}\,X^{(2)}_1(t)+A^{(2)}_{3,2}\,X^{(2)}_2(t)+A^{(2)}_{3,3}\,X^{(2)}_3(t)\Big) &= G(X^{(2)}_3(t)) \\
&= X^{(2)}_3(t)\,v_0\,e^{-n\,X^{(2)}_3(t)}
\end{aligned} \tag{98}$$

Finally, we write the element boundary conditions. We have just one pair, since there is only one interior node (H_2):

$$\begin{aligned}
X^{(2)}_0(t) &= X^{(1)}_2(t)\,; \\
\frac{1}{L\,\Delta_2}\sum_{k=0}^{3} A^{(2)}_{0,k}\,X^{(2)}_k(t) &= \frac{1}{L\,\Delta_1}\sum_{k=0}^{2} A^{(1)}_{2,k}\,X^{(1)}_k(t)\,.
\end{aligned} \tag{99}$$

Expanding the second of the two equations above, we have:

$$\begin{aligned}
&\frac{1}{L\,\Delta_2}\Big(A^{(2)}_{0,0}\,X^{(2)}_0(t)+A^{(2)}_{0,1}\,X^{(2)}_1(t)+A^{(2)}_{0,2}\,X^{(2)}_2(t)+A^{(2)}_{0,3}\,X^{(2)}_3(t)\Big) = \\
&\quad\frac{1}{L\,\Delta_1}\Big(A^{(1)}_{2,0}\,X^{(1)}_0(t)+A^{(1)}_{2,1}\,X^{(1)}_1(t)+A^{(1)}_{2,2}\,X^{(1)}_2(t)\Big)\,.
\end{aligned} \tag{100}$$

Thus the set of $N_T = 7$ equations we have to solve for the seven unknown concentration values $\{X^{(1)}_0(t), ...X^{(2)}_3(t)\}$ are: the three DAEs - Eqns.(92), (94), (95) with the three initial conditions - Eqns.(96) ; the two boundary conditions given by Eqns.(98) and the two element continuity conditions, Eqns.(100).

8.2 Matrix formulation

One way to solve the DAEs - Eqns.(92-95), is to use matrices to represent the unknown concentrations at the nodes and interior collocation points [6]. The associated domain boundary conditions and the element boundary conditions can also be combined and written in matrix form. In addition, there are the collocation matrices A and B over each element. If we have only linear terms appearing in the DAEs, we can finally even write the entire set of DAEs as a matrix equation. In our case, though, we do have non-linear terms in all the DAEs. However, we can still employ matrices to eliminate the unknowns at the nodes, to yield a coupled set of DAEs involving only the unknowns at the interior collocation points. We illustrate this procedure below.

Let us first define two vectors W and U, which are the vectors of unknown concentrations at the internal collocation points and at the nodes respectively. That is,

$$W \equiv \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} \equiv \begin{bmatrix} X_1^{(1)}(t) \\ X_1^{(2)}(t) \\ X_2^{(2)}(t) \end{bmatrix} \tag{101}$$

and

$$U \equiv \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \equiv \begin{bmatrix} X_0^{(1)}(t) \\ X_2^{(1)}(t) = X_0^{(2)}(t) \\ X_3^{(2)}(t) \end{bmatrix} . \tag{102}$$

We also define the vector of initial values at the interior collocation points:

$$W^0 \equiv \begin{bmatrix} w_1^0 \\ w_2^0 \\ w_3^0 \end{bmatrix} \equiv \begin{bmatrix} X_1^{(1)}(t=0) \\ X_1^{(2)}(t=0) \\ X_2^{(2)}(t=0) \end{bmatrix} \tag{103}$$

Note that in defining U, we have already used the first of Eqns.(100). In general, the vectors W and W^0 have the dimension $[\,N_C \times 1]$, and U is of dimension $[\,(N_E+1) \times 1\,]$.

Thus the DAEs are written for the $\{w_i\}$, the unknown concentrations at the interior collocation points:

$$\begin{aligned} \frac{dw_1}{dt} \quad = \quad & \Big[-a_1\, g(w_1)\, A_{1,1}^{(1)} + c_1\, B_{1,1}^{(1)}\Big]\; w_1 \\ & + \Big[-a_1\, g(w_1)\, A_{1,0}^{(1)} + c_1\, B_{1,0}^{(1)}\Big]\; u_1 \\ & + \Big[-a_1\, g(w_1)\, A_{1,2}^{(1)} + c_1\, B_{1,2}^{(1)}\Big]\; u_2\, ; \end{aligned} \tag{104}$$

$$\begin{aligned} \frac{dw_2}{dt} \quad = \quad & \Big[-a_2\, g(w_2)\, A_{1,1}^{(2)} + c_2\, B_{1,1}^{(2)}\Big]\; w_2 \\ & + \Big[-a_2\, g(w_2)\, A_{1,2}^{(2)} + c_2\, B_{1,2}^{(2)}\Big]\; w_3 \\ & + \Big[-a_2\, g(w_2)\, A_{1,0}^{(2)} + c_2\, B_{1,0}^{(2)}\Big]\; u_2 \\ & + \Big[-a_2\, g(w_2)\, A_{1,3}^{(2)} + c_2\, B_{1,3}^{(2)}\Big]\; u_3\, ; \end{aligned} \tag{105}$$

and:

$$\begin{aligned} \frac{dw_3}{dt} \quad = \quad & \Big[-a_2\, g(w_3)\, A_{2,1}^{(2)} + c_2\, B_{2,1}^{(2)}\Big]\; w_2 \\ & + \Big[-a_2\, g(w_3)\, A_{2,2}^{(2)} + c_2\, B_{2,2}^{(2)}\Big]\; w_3 \\ & + \Big[-a_2\, g(w_3)\, A_{2,0}^{(2)} + c_2\, B_{2,0}^{(2)}\Big]\; u_2 \\ & + \Big[-a_2\, g(w_3)\, A_{2,3}^{(2)} + c_2\, B_{2,3}^{(2)}\Big]\; u_3\, ; \end{aligned} \tag{106}$$

In the equations above, we have used the convenient notation:

$$\begin{array}{rr} 1/L\,\Delta_1 = a_1\, ; & 1/L\,\Delta_2 = a_2\, ; \\ D_0/L\,\Delta_1 = b_1\, ; & D_0/L\,\Delta_2 = b_2\, ; \\ D_0/L^2\,\Delta_1^2 = c_1\, ; & D_0/L^2\,\Delta_2^2 = c_2\, ; \end{array} \tag{107}$$

and the function:

$$g(x) \;=\; \frac{(1-n\,x)}{x}\,G(x) = \;(1-n\,x)\,v_o\,e^{-n\,x}\,. \tag{108}$$

We see from Eqns.(104-106) above that their right hand sides contain terms involving both the $\{w_i\}$, and the $\{u_i\}$, which are the unknown concentrations at the element boundaries (nodes). The easiest way to solve the DAEs is to eliminate the $\{u_i\}$, by writing them in terms of the $\{w_i\}$. This can be done if we can explicitly relate the $\{u_i\}$ and the $\{w_i\}$. We can try to do this using the algebraic relations, Eqns.(98) and Eqns.(100), describing the boundary conditions and continuity at the elements.

We can write Eqns.(98) and the second of Eqns.(100) in terms of the $\{w_i\}$ and $\{u_i\}$. Re-ordering the equations, we have :

$$\begin{aligned}
b_1\,A^{(1)}_{0,1}\,w_1 \;&=\; \left(v_0 e^{-n\,u_1} - b_1\,A^{(1)}_{0,0}\right)\,u_1 - b_1 A^{(1)}_{0,2}\,u_2\,; \\
-a_1\,A^{(1)}_{2,1}\,w_1 + a_2\,A^{(2)}_{0,1}\,w_2 + a_2\,A^{(2)}_{0,2}\,w_3 \;&=\; a_1\,A^{(1)}_{2,0}\,u_1 + (a_1\,A^{(1)}_{2,2} - a_2\,A^{(2)}_{0,0})\,u_2 - a_2\,A^{(2)}_{0,3}\,u_3\,; \\
b_2\,A^{(2)}_{3,1}\,w_2 + b_2\,A^{(2)}_{3,2}\,w_3 \;&=\; -b_2\,A^{(2)}_{3,0}\,u_2 + \left(v_0 e^{-n\,u_3} - b_2\,A^{(2)}_{3,3}\right)\,u_3\,.
\end{aligned} \tag{109}$$

We can simply write the above equations together in matrix form, if we linearize the exponential terms in the boundary conditions. That is, as a first approximation, we replace $(e^{-n\,u_1},\, e^{-n\,u_3})$ by 1, the first term in their Taylor expansion. We can then write the matrix equation:

$$P\,W = Q\,U\,. \tag{110}$$

The matrices P and Q are given by:

$$P \equiv \begin{bmatrix} b_1\,A^{(1)}_{0,1} & 0 & 0 \\ -a_1\,A^{(1)}_{2,1} & a_2\,A^{(2)}_{0,1} & a_2\,A^{(2)}_{0,2} \\ 0 & b_2\,A^{(2)}_{3,1} & b_2\,A^{(2)}_{3,2} \end{bmatrix}\,. \tag{111}$$

Note that P has the dimension $[\,(N_E+1)\times N_C\,]$. Now Q has the form:

$$Q \equiv \begin{bmatrix} (\,v_0 - b_1\,A^{(1)}_{0,0}\,) & -b_1\,A^{(1)}_{0,2} & 0 \\ a_1\,A^{(1)}_{2,0} & (\,a_1\,A^{(1)}_{2,2} - a_2\,A^{(2)}_{0,0}\,) & -a_2\,A^{(2)}_{0,3} \\ 0 & -b_2\,A^{(2)}_{3,0} & (\,v_0 - b_2\,A^{(2)}_{3,3}\,) \end{bmatrix}\,. \tag{112}$$

Notice that Q is a square tridiagonal matrix of dimension $[\,(N_E+1)\times(N_E+1)\,]$.

We can solve for U from Eq.(110):

$$U = Q^{-1}\,P\,W\,; \tag{113}$$

or, defining a matrix $R \equiv Q^{-1}\,P$ we have:

$$U = R\,W\,. \tag{114}$$

This is the required equation relating U and W. We first obtain R, and can then substitute for the $\{u_i\}$ appearing in Eqns.(104-106) in terms of the $\{w_i\}$, thus yielding a coupled system of DAEs in the $\{w_i\}$. Solving these, together with the initial conditions given by Eq.(103), we obtain W. We then obtain U explicitly from Eq.(114). Thus W and U together constitute the full solution of the PDE.

8.3 An example for continuous sedimentation

For the continuous sedimentation case, we divide the domain of interest $[0, 1]$ into *three* elements, by defining four nodes $\{ H_1 = 0, H_2 = 0.3, H_3 = 0.4, H_4 = 1.0 \}$. We locate the rectangular unit pulse representing the delta function source on the second element. We locate one interior collocation point each on the first and second elements, and two on the third. The parameters of the problem are therfore:

$$\begin{aligned}
\alpha &= 0\,; \\
\beta &= 0\,; \\
N_E &= 3\,; \\
i &= 1,\,2,\,3 \\
\Delta_1 &= (H_2 - H_1) = 0.3\,; \\
\Delta_2 &= (H_3 - H_2) = 0.1 = 2\sigma\,; \\
\Delta_3 &= (H_4 - H_3) = 0.6\,; \\
N(1) &= 1\,; \\
N(2) &= 1\,; \\
N(3) &= 2\,; \\
N_C &= 4\,; \\
N_T &= 10\,;
\end{aligned} \tag{115}$$

Now the appropriate Jacobi polynomials are, respectively for the three elements, $(\, G_1(0, 0, x),\ G_1(0, 0, x),\ G_2(0, 0, x)\,)$. We have already evaluated these polynomials and their roots for the batch case.

The collocation points $\{\xi_j^{(i)}\}$ are given by:

$$\begin{aligned}
\xi_0^{(1)} &= 0.0\,; \\
\xi_1^{(1)} &= 0.5\,; \\
\xi_2^{(1)} &= 1.0\,; \\
\xi_0^{(2)} &= 0.0\,; \\
\xi_1^{(2)} &= 0.5\,; \\
\xi_2^{(2)} &= 1.0\,; \\
\xi_0^{(3)} &= 0.0\,; \\
\xi_1^{(3)} &= 0.21132\,; \\
\xi_2^{(3)} &= 0.78868\,; \\
\xi_3^{(3)} &= 1.0\,;
\end{aligned} \tag{116}$$

The corresponding Lagrange polynomials follow:

$$p_1(\xi^{(1)}) = (\xi^{(1)} - 0.0)\,(\xi^{(1)} - 0.5)\,(\xi^{(1)} - 1.0)\,; \tag{117}$$

$$p_2(\xi^{(2)}) = (\xi^{(2)} - 0.0)\,(\xi^{(2)} - 0.5)\,(\xi^{(2)} - 1.0)\,; \tag{118}$$

and

$$p_3(\xi^{(3)}) = (\xi^{(3)} - 0.0)\,(\xi^{(3)} - 0.21132)\,(\xi^{(3)} - 0.78868)\,(\xi^{(3)} - 1.0)\,. \tag{119}$$

The collocation matrices are now given by:

$$A^{(1)} = A^{(2)} \equiv \begin{bmatrix} -3.0 & 4.0 & -1.0 \\ -1.0 & 0.0 & 1.0 \\ 1.0 & -4.0 & 3.0 \end{bmatrix} ; \tag{120}$$

$$B^{(1)} = B^{(2)} \equiv \begin{bmatrix} 4.0 & -8.0 & 4.0 \\ 4.0 & -8.0 & 4.0 \\ 4.0 & -8.0 & 4.0 \end{bmatrix} ; \tag{121}$$

$$A^{(3)} \equiv \begin{bmatrix} -7.00000 & 8.19615 & -2.19615 & 1.00000 \\ -2.73205 & 1.73205 & 1.73205 & -0.73205 \\ 0.73205 & -1.73205 & -1.73205 & 2.73205 \\ -1.00000 & 2.19615 & -8.19615 & 7.00000 \end{bmatrix} ; \tag{122}$$

$$B^{(3)} \equiv \begin{bmatrix} 24.00000 & -37.17691 & 25.17691 & -12.00000 \\ 16.39230 & -24.00000 & 12.00000 & -4.39230 \\ -4.39230 & 12.00000 & -24.00000 & 16.39230 \\ -12.00000 & 25.17691 & -37.17691 & 24.00000 \end{bmatrix} . \tag{123}$$

We can now write down explicitly the DAEs for the concentration at the $N_C = 4$ interior collocation points, Eqns.(66,67, 68).

For the collocation point $\xi_1^{(1)}$ within the first element, we have:

$$\frac{dX_1^{(1)}(t)}{dt} = \sum_{k=0}^{2} \left[-\frac{1}{L\Delta_1} \left(\left(1 - n\,X_1^{(1)}(t)\right)\; v_0\; e^{-n\,X_1^{(1)}(t)} + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A} \right) A_{1,k}^{(1)} + \frac{D_0}{L^2\Delta_1^2}\, B_{1,k}^{(1)} \right] X_k^{(1)}(t). \tag{124}$$

For the collocation point $\xi_1^{(2)}$ within the second element, we have:

$$\begin{aligned} \frac{dX_1^{(2)}(t)}{dt} &= \sum_{k=0}^{2} \left[-\frac{1}{L\Delta_2} \left(\left(1 - n\,X_1^{(2)}(t)\right)\; v_0\; e^{-n\,X_1^{(2)}(t)} + \frac{Q_u(t)}{A} \right) A_{1,k}^{(2)} + \frac{D_0}{L^2\Delta_2^2}\, B_{1,k}^{(2)} \right] X_k^{(2)}(t) \\ &\quad - \left(X_1^{(2)}(t) \;+\; X_f(t) \right) \frac{Q_f(t)}{A} . \end{aligned} \tag{125}$$

At the two interior collocation points $(\xi_1^{(3)}, \xi_2^{(3)})$, we have the DAEs:

$$\frac{dX_1^{(3)}(t)}{dt} = \sum_{k=0}^{3} \left[-\frac{1}{L\Delta_3} \left(\left(1 - n\,X_1^{(3)}(t)\right)\; v_0\; e^{-n\,X_1^{(3)}(t)} + \frac{Q_u(t)}{A} \right) A_{1,k}^{(3)} + \frac{D_0}{L^2\Delta_3^2}\, B_{1,k}^{(3)} \right] X_k^{(3)}(t)\,; \tag{126}$$

$$\frac{dX_2^{(3)}(t)}{dt} = \sum_{k=0}^{3} \left[-\frac{1}{L\Delta_3} \left(\left(1 - n\,X_2^{(3)}(t)\right)\; v_0\; e^{-n\,X_2^{(3)}(t)} + \frac{Q_u(t)}{A} \right) A_{2,k}^{(3)} + \frac{D_0}{L^2\Delta_3^2}\, B_{2,k}^{(3)} \right] X_k^{(3)}(t)\,. \tag{127}$$

The four DAEs above (Eqns.(124)-(127)) must be solved together with the initial conditions:

$$\begin{aligned} X_1^{(1)}(t=0) &= X_{10}^{(1)} = X_0\,; \\ X_1^{(2)}(t=0) &= X_{10}^{(2)} = X_0\,; \\ X_1^{(3)}(t=0) &= X_{10}^{(3)} = X_0\,; \\ X_2^{(3)}(t=0) &= X_{20}^{(3)} = X_0\,. \end{aligned} \tag{128}$$

The two boundary conditions (at $z = 0, L$) are now given by the equations:

$$\begin{aligned} \frac{D_0}{L\,\Delta_1} \sum_{k=0}^{2} A_{0,k}^{(1)}\,X_k^{(1)}(t) &= 0\,; \\ \frac{D_0}{L\,\Delta_3} \sum_{k=0}^{3} A_{3,k}^{(3)}\,X_k^{(3)}(t) &= 0\,. \end{aligned} \tag{129}$$

Expanding them, we have:

$$\begin{aligned} \frac{D_0}{L\,\Delta_1} \left(A_{0,0}^{(1)}\,X_0^{(1)}(t) + A_{0,1}^{(1)}\,X_1^{(1)}(t) + A_{0,2}^{(1)}\,X_2^{(1)}(t) \right) &= 0\,; \\ \frac{D_0}{L\,\Delta_3} \left(A_{3,0}^{(3)}\,X_0^{(3)}(t) + A_{3,1}^{(3)}\,X_1^{(3)}(t) + A_{3,2}^{(3)}\,X_2^{(3)}(t) + A_{3,3}^{(3)}\,X_3^{(3)}(t) \right) &= 0\,. \end{aligned} \tag{130}$$

Finally, we write the element boundary conditions. We now have two pairs, since there are two interior nodes (H_2, H_3):

$$\begin{aligned} X_0^{(2)}(t) &= X_2^{(1)}(t)\,; \\ X_0^{(3)}(t) &= X_2^{(2)}(t)\,; \\ \frac{1}{L\,\Delta_2} \sum_{k=0}^{2} A_{0,k}^{(2)}\,X_k^{(2)}(t) &= \frac{1}{L\,\Delta_1} \sum_{k=0}^{2} A_{2,k}^{(1)}\,X_k^{(1)}(t) \\ \frac{1}{L\,\Delta_3} \sum_{k=0}^{3} A_{0,k}^{(3)}\,X_k^{(3)}(t) &= \frac{1}{L\,\Delta_2} \sum_{k=0}^{2} A_{2,k}^{(2)}\,X_k^{(2)}(t)\,. \end{aligned} \tag{131}$$

Expanding the last two of the equations above, we have:

$$\begin{aligned} &\frac{1}{L\,\Delta_2} \left(A_{0,0}^{(2)}\,X_0^{(2)}(t) + A_{0,1}^{(2)}\,X_1^{(2)}(t) + A_{0,2}^{(2)}\,X_2^{(2)}(t) \right) = \\ &\qquad \frac{1}{L\,\Delta_1} \left(A_{2,0}^{(1)}\,X_0^{(1)}(t) + A_{2,1}^{(1)}\,X_1^{(1)}(t) + A_{2,2}^{(1)}\,X_2^{(1)}(t) \right)\;; \end{aligned}$$

and:

$$\begin{aligned} &\frac{1}{L\,\Delta_3} \left(A_{0,0}^{(3)}\,X_0^{(3)}(t) + A_{0,1}^{(3)}\,X_1^{(3)}(t) + A_{0,2}^{(3)}\,X_2^{(3)}(t) + A_{0,3}^{(3)}\,X_3^{(3)}(t) \right) = \\ &\qquad \frac{1}{L\,\Delta_2} \left(A_{2,0}^{(2)}\,X_0^{(2)}(t) + A_{2,1}^{(2)}\,X_1^{(2)}(t) + A_{2,2}^{(2)}\,X_2^{(2)}(t) \right)\,. \end{aligned} \tag{132}$$

Thus for the continuous case, the set of $N_T = 10$ equations we have to solve for the ten unknown concentration values $\{X_0^{(1)}(t), ...X_3^{(3)}(t)\}$ are: the four DAEs - Eqns.(124)-(127) with the four initial conditions - Eqns.(128) ; the two boundary conditions given by Eqns.(130) and the four element continuity conditions, Eqns.(131).

8.4 Matrix formulation

We shall again solve the DAEs for the continous case, Eqns.(124-127) using matrices. The vectors of unknown concentrations at the interior collocation points and at the nodes, W and U are:

$$W \equiv \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} \equiv \begin{bmatrix} X_1^{(1)}(t) \\ X_1^{(2)}(t) \\ X_1^{(3)}(t) \\ X_2^{(3)}(t) \end{bmatrix} \tag{133}$$

and

$$U \equiv \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} \equiv \begin{bmatrix} X_0^{(1)}(t) \\ X_2^{(1)}(t) = X_0^{(2)}(t) \\ X_2^{(2)}(t) = X_0^{(3)}(t) \\ X_3^{(3)}(t) \end{bmatrix} . \tag{134}$$

The vector of initial values at the interior collocation points is:

$$W^0 \equiv \begin{bmatrix} w_1^0 \\ w_2^0 \\ w_3^0 \\ w_4^0 \end{bmatrix} \equiv \begin{bmatrix} X_1^{(1)}(t=0) \\ X_1^{(2)}(t=0) \\ X_1^{(3)}(t=0) \\ X_2^{(3)}(t=0) \end{bmatrix} \tag{135}$$

The DAEs are written for the $\{w_i\}$:

$$\begin{aligned} \frac{dw_1}{dt} \quad = \quad & \left[-a_1 \left(g(w_1) + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A} \right) A_{1,1}^{(1)} + c_1 \, B_{1,1}^{(1)} \right] w_1 \\ & + \left[-a_1 \left(g(w_1) + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A} \right) A_{1,0}^{(1)} + c_1 \, B_{1,0}^{(1)} \right] u_1 \\ & + \left[-a_1 \left(g(w_1) + \frac{Q_u(t)}{A} - \frac{Q_f(t)}{A} \right) A_{1,2}^{(1)} + c_1 \, B_{1,2}^{(1)} \right] u_2 \, ; \end{aligned} \tag{136}$$

$$\begin{aligned} \frac{dw_2}{dt} \quad = \quad & \left[-a_2 \left(g(w_2) + \frac{Q_u(t)}{A} \right) A_{1,1}^{(2)} + c_2 \, B_{1,1}^{(2)} \right] w_2 \\ & + \left[-a_2 \left(g(w_2) + \frac{Q_u(t)}{A} \right) A_{1,0}^{(2)} + c_2 \, B_{1,0}^{(2)} \right] u_2 \\ & + \left[-a_2 \left(g(w_2) + \frac{Q_u(t)}{A} \right) A_{1,2}^{(2)} + c_2 \, B_{1,2}^{(2)} \right] u_3 \\ & - (\, w_2 + X_f(t) \,) \, \frac{Q_f(t)}{A}; \end{aligned} \tag{137}$$

$$\begin{aligned} \frac{dw_3}{dt} \quad = \quad & \left[-a_3 \left(g(w_3) + \frac{Q_u(t)}{A} \right) A_{1,1}^{(3)} + c_3 \, B_{1,1}^{(3)} \right] w_3 \\ & + \left[-a_3 \left(g(w_3) + \frac{Q_u(t)}{A} \right) A_{1,2}^{(3)} + c_3 \, B_{1,2}^{(3)} \right] w_4 \\ & + \left[-a_3 \left(g(w_3) + \frac{Q_u(t)}{A} \right) A_{1,0}^{(3)} + c_3 \, B_{1,0}^{(3)} \right] u_3 \\ & + \left[-a_3 \left(g(w_3) + \frac{Q_u(t)}{A} \right) A_{1,3}^{(3)} + c_3 \, B_{1,3}^{(3)} \right] u_4 \, ; \end{aligned} \tag{138}$$

and:

$$\begin{aligned}
\frac{dw_4}{dt} \quad = \quad & \left[-a_3 \left(g(w_4)+\frac{Q_u(t)}{A}\right) A^{(3)}_{2,1} + c_3\, B^{(3)}_{2,1}\right] w_3 \\
& + \left[-a_3 \left(g(w_4)+\frac{Q_u(t)}{A}\right) A^{(2)}_{2,2} + c_3\, B^{(3)}_{2,2}\right] w_4 \\
& + \left[-a_3 \left(g(w_4)+\frac{Q_u(t)}{A}\right) A^{(3)}_{2,0} + c_3\, B^{(3)}_{2,0}\right] u_3 \\
& + \left[-a_3 \left(g(w_4)+\frac{Q_u(t)}{A}\right) A^{(3)}_{2,3} + c_3\, B^{(3)}_{2,3}\right] u_4\,;
\end{aligned} \tag{139}$$

In the equations above, we have used the convenient notation:

$$\begin{array}{rrr}
1/L\,\Delta_1 = a_1\,; & 1/L\,\Delta_2 = a_2 & 1/L\,\Delta_3 = a_3\,; \\
D_0/L\,\Delta_1 = b_1\,; & D_0/L\,\Delta_2 = b_2 & D_0/L\,\Delta_3 = b_3\,; \\
D_0/L^2\,\Delta_1^2 = c_1\,; & D_0/L^2\,\Delta_2^2 = c_2 & D_0/L^2\,\Delta_3^2 = c_3\,;
\end{array} \tag{140}$$

and the function $g(x)$ is as defined before for the batch case:

$$g(x) \;=\; (1-n\,x)\,v_o\,e^{-n\,x}; \tag{141}$$

The algebraic equations resulting from the boundary conditions and the element continuity conditions are as follows:

$$\begin{aligned}
A^{(1)}_{0,1}\,w_1 \quad &= \quad -A^{(1)}_{0,0}\,u_1 - A^{(1)}_{0,2}\,u_2\,; \\
-a_1\,A^{(1)}_{2,1}\,w_1 + a_2\,A^{(2)}_{0,1}\,w_2 \quad &= \quad a_1\,A^{(1)}_{2,0}\,u_1 + (a_1\,A^{(1)}_{2,2} - a_2\,A^{(2)}_{0,0})\,u_2\; - a_2\,A^{(2)}_{0,2}\,u_3\,; \\
-a_2\,A^{(2)}_{2,1}\,w_2 + a_3\,A^{(3)}_{0,1}\,w_3 + a_3\,A^{(3)}_{0,2}\,w_4 \quad &= \quad a_2\,A^{(2)}_{2,0}\,u_2 + (a_2\,A^{(2)}_{2,2} - a_3\,A^{(3)}_{0,0})\,u_3 - a_3\,A^{(3)}_{0,3}\,u_4\,; \\
A^{(3)}_{3,1}\,w_3 + A^{(3)}_{3,2}\,w_4 \quad &= \quad -A^{(3)}_{3,0}\,u_3 - A^{(3)}_{3,3}\,u_4\,.
\end{aligned} \tag{142}$$

The equations above are all linear. Thus the matrices P and Q are given by:

$$P \equiv \begin{bmatrix}
A^{(1)}_{0,1} & 0 & 0 & 0 \\
-a_1\,A^{(1)}_{2,1} & a_2\,A^{(2)}_{0,1} & 0 & 0 \\
0 & -a_2\,A^{(2)}_{2,1} & a_3\,A^{(3)}_{0,1} & a_3\,A^{(3)}_{0,2} \\
0 & 0 & A^{(3)}_{3,1} & A^{(3)}_{3,2}
\end{bmatrix}. \tag{143}$$

And Q has the form:

$$Q \equiv \begin{bmatrix}
-A^{(1)}_{0,0}\,) & -A^{(1)}_{0,2} & 0 & 0 \\
a_1\,A^{(1)}_{2,0} & (\,a_1\,A^{(1)}_{2,2} - a_2\,A^{(2)}_{0,0}\,) & -a_2\,A^{(2)}_{0,2} & 0 \\
0 & a_2\,A^{(2)}_{2,0} & (\,a_2\,A^{(2)}_{2,2} - a_3\,A^{(3)}_{0,0}\,) & -a_3\,A^{(3)}_{0,3} \\
0 & 0 & -A^{(3)}_{3,0} & -A^{(3)}_{3,3}
\end{bmatrix}. \tag{144}$$

We can thus find the matrix $R \equiv Q^{-1} P$, and hence obtain the required coupled set of DAEs in the $\{w_i\}$. Solving these, and using the relation $U = RW$, we finally obtain the full solution of the original PDE for continuous sedimentation, Eqns.(62-64).

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