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March 6, 1990

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1 Introduction

The paper [1] by Hindmarsh and Johnson discusses the formulation and solution of certain reaction-diffusion systems involving Stefan-Maxwell diffusion. This report is intended to provide supportive analytical results concerning the systems of differential-algebraic equations (DAEs) treated in that paper. The systems considered have only one reactant fluid, one product fluid, and one reactant solid; this restricted problem was chosen because the various solvability issues can be settled quite thoroughly. Of particular interest is the index of the DAE systems, the evaluation of consistent initial conditions, and the conservation of the sum of fluid mole fractions.

As developed in [1], the normalized isothermal flux model of interest is given by the following continuous equations (see (4.11) in [1]) in time t and radius η ($0 \leq \eta \leq 1$):

$$\left.\begin{aligned} \partial x_1/\partial t &= S_1 - \gamma \nabla \cdot n_1 \\ \partial x_2/\partial t &= S_2 - \gamma \nabla \cdot n_2 \\ \nabla x_1 &= x_1 n_2 - x_2 n_1 \\ \nabla x_2 &= x_2 n_1 - x_1 n_2 \\ \partial w/\partial t &= S_3 \,. \end{aligned}\right\} \tag{1.1}$$

For simplicity, the notation here is changed slightly from that in [1]: Subscripts A, P, and B have been replaced by 1, 2, and 3, and the asterisks (representing normalized coordinates) have been dropped. In the next three sections, a discretized form of (1.1) and an altered version of that model are presented and analyzed. The main results are that the initial semi-discrete model has index 2 and is solvable, but does not conserve the mole-fraction sum $x_1 + x_2$, while the altered model (with a mild assumption on the spatial mesh) also has index 2 and is solvable, and does conserve $x_1 + x_2$.

The fluxless form of the same model (see (5.7) in [1]) is given by

$$\left.\begin{aligned} \partial x_1/\partial t &= S_1 - x_1 S - \gamma \nu x_{1\eta} + \gamma \nabla^2 x_1 \\ \partial x_2/\partial t &= S_2 - x_2 S - \gamma \nu x_{2\eta} + \gamma \nabla^2 x_2 \\ \partial w/\partial t &= S_3 \\ \gamma \nabla \cdot (\nu \underline{r}) &= S \equiv S_1 + S_2 \,. \end{aligned}\right\} \tag{1.2}$$

Here the subscript η denotes differentiation. A semi-discrete form of (1.2) is shown to be solvable and have index 1, and to guarantee conservation of $x_1 + x_2$.

It is worth noting that the discrete fluxless model is obtained from continuous equations (1.2) representing flux elimination operations on the original continuous equations (1.1), and this is *not* the same as discretizing first and then eliminating fluxes. The latter could be considered, but (among other drawbacks) it would involve the product of a discrete divergence and a discrete gradient operator, as compared to a discrete form of the Laplacian operator defined directly.

We believe that the analysis of these discrete isothermal models can be extended in a straightforward manner to the non-isothermal case, though this has not been carried out. The initial non-isothermal model has an additional term in each fluid equation as well as the additional evolution equation for temperature. But these differences would not appear to interfere in any way with the index and conservation analysis as done in the isothermal case.

Likewise, the analysis should extend to multi-species models. However, only the fluxless DAE form, generalizing (1.2), has been adopted for computation, as discussed in [2] and [3]. The discrete form of this model is clearly solvable and of index 1 by inspection, and it appears that fluid conservation can be easily established for it also.

2 The Initial Model

We first study the original isothermal model, discretized on a mesh of M intervals, with mesh points η_j $(j = 0, 1, \ldots, M)$, such that $\eta_0 = 1$, $\eta_M = 1$. Denote the dependent variable vector by

$$y = (x_1, x_2, w, n_1, n_2)^T,$$

where each block above has $M + 1$ components x_1^j etc., associated with mesh points η_j. We write the equations for the model as

$$\left.\begin{array}{rcl} \dot{x}_1 & = & S_1 - \gamma D n_1 \equiv g_1 \\ \dot{x}_2 & = & S_2 - \gamma D n_2 \equiv g_2 \\ \dot{w} & = & S_3 \equiv g_3 \\ 0 & = & I_0 n_1 + E_2 n_1 - E_1 n_2 + G x_1 + b_1 \equiv g_4 \\ 0 & = & I_0 n_2 + E_1 n_2 - E_2 n_1 + G x_2 + b_2 \equiv g_5. \end{array}\right\} \qquad (2.1)$$

Here the S_k are vectors of source functions, whose details are irrelevant here. D is a square matrix of order $M + 1$ representing the discrete divergence operator. $I_0 = \mathrm{diag}(1, 0, \ldots, 0)$ is introduced so that $I_0 n_k = 0$ represents the condition $n_k^0 = 0$. The matrices E_1 and E_2 are defined by $E_k = \mathrm{diag}(0, x_k^1, \ldots, x_k^M)$ $(k = 1, 2)$. G is a square matrix of order $M + 1$ which represents the discrete gradient operation in its internal rows. Its first row (row 0) is all zeros, and its last row is zero except for its last diagonal element, which is $-Sh$. The vector b_k, of length $M + 1$, has a last component of $Sh\, x_{kb}$ (x_{kb} = bulk value of x_k), and all other components equal to zero. Thus $G x_k + b_k$ is the discrete gradient of x_k at all points, including boundary conditions.

We write this system more concisely by defining a matrix of order $5(M + 1)$ in block form,

$$A = \begin{bmatrix} I & & & & \\ & I & & & \\ & & I & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix}$$

(I is the identity matrix of size $M + 1$), and a vector g with 5 blocks, g_1 to g_5. Thus the system (2.1) is simply

$$A\dot{y} = g(y). \qquad (2.2)$$

The index analysis for (2.2) begins with the observation that the original system has a differential part (the first three blocks) and a nontrivial algebraic part (the rest). Hence its index is clearly greater than 0.

The next step is to differentiate the algebraic part of (2.2) and manipulate the result so as to maximize the number of zero rows in the matrix multiplying $\dot{y}$. To represent the result compactly, define another pair of diagonal matrices,

$$\begin{aligned} N_1 &= \operatorname{diag}(0, n_1^1, \ldots, n_1^M) \\ N_2 &= \operatorname{diag}(0, n_2^1, \ldots, n_2^M). \end{aligned}$$

Then the equation $\dot{g}_4 = 0$ becomes

$$G\dot{x}_1 - N_2\dot{x}_1 + N_1\dot{x}_2 + (E_2 + I_0)\dot{n}_1 - E_1\dot{n}_2 = 0$$

and $\dot{g}_5 = 0$ becomes

$$N_2\dot{x}_1 + G\dot{x}_2 - N_1\dot{x}_2 - E_2\dot{n}_1 + (E_1 + I_0)\dot{n}_2 = 0.$$

The system thus has the form

$$A^{(1)}\dot{y} = g^{(1)} = (g_1, g_2, g_3, 0, 0)^T, \tag{2.3}$$

where

$$A^{(1)} = \begin{bmatrix} I & & & & \\ & I & & & \\ & & I & & \\ G - N_2 & N_1 & 0 & E_2 + I_0 & -E_1 \\ N_2 & G - N_1 & 0 & -E_2 & E_1 + I_0 \end{bmatrix}.$$

(Blanks represent zero blocks.)

The last two block-rows in the system (2.3) have much in common. This allows us to do simple operations which separate the system into differential and algebraic parts. First, if we add block-row 4 (excluding row 0) to block-row 5 (excluding row 0), the last block-row of $A^{(1)}$ becomes

$$(G, G, 0, 0, I_0),$$

while the last block of $g^{(1)}$ remains 0. Next, the blocks equal to G above can be eliminated by adding $-G$ times block-rows 1 and 2 to the last block-row. The resulting system is

$$A^{(2)}\dot{y} = g^{(2)} = (g_1, g_2, g_3, 0, -G(g_1 + g_2))^T, \tag{2.4}$$

where

$$A^{(2)} = \begin{bmatrix} I & & & & \\ & I & & & \\ & & I & & \\ G - N_2 & N_1 & 0 & E_2 + I_0 & -E_1 \\ 0 & 0 & 0 & 0 & I_0 \end{bmatrix}.$$

In this form, the system has M algebraic equations (the last M equations), and the rest is a differential system. Before proceeding, we must be sure that we cannot get a larger number of algebraic equations by such manipulations. The blocks equal to $G - N_2$ and N_1 in block-row 4 of $A^{(2)}$ can be eliminated by use of the first two block-rows. This would leave a matrix that looks like the identity matrix except for the square block

$$\begin{bmatrix} E_2 + I_0 & -E_1 \\ 0 & I_0 \end{bmatrix}$$

of size $2(M+1)$. As long as all $x_1^j + x_2^j > 0$, this matrix has rank $M+2$, since elementary column operations on it give

$$\begin{bmatrix} E_1 + E_2 + I_0 & -E_1 \\ 0 & I_0 \end{bmatrix}$$

with $E_1 + E_2 + I_0 = \mathrm{diag}(1,\, x_1^1 + x_2^1,\, \ldots,\, x_1^M + x_2^M)$. This means that at most $2(M+1) - (M+2) = M$ rows of $A^{(2)}$ can be zeroed out.

Since one differentiation of the system has still left an algebraic part in it, the index of the original system is ≥ 2, and we must differentiate the algebraic part of $A^{(2)}\dot{y} = g^{(2)}$ to determine the index. To represent that part, let $\bar{G}$ denote the $M \times (M+1)$ matrix which is G with row 0 removed. Then the algebraic system in (2.4) (with a change in sign) can be written

$$0 = \bar{G}(g_1 + g_2) = \bar{G}\left[S_1 + S_2 - \gamma D(n_1 + n_2)\right].$$

We differentiate this, getting a system

$$\bar{G}\left[\frac{\partial S}{\partial x_1}\dot{x}_1 + \frac{\partial S}{\partial x_2}\dot{x}_2 + \frac{\partial S}{\partial w}\dot{w} - \gamma D(\dot{n}_1 + \dot{n}_2)\right] = 0$$

where $S \equiv S_1 + S_2$. The new system is therefore

$$A^{(3)}\dot{y} = g^{(3)} = (g_1,\, g_2,\, g_3,\, 0,\, 0)^T, \tag{2.5}$$

where

$$A^{(3)} = \begin{bmatrix} I & & & & \\ & I & & & \\ & & I & & \\ G - N_2 & N_1 & 0 & E_2 + I_0 & -E_1 \\ 0 & 0 & 0 & 0 & e_0^T \\ J_1 & J_2 & J_3 & -\gamma \bar{G} D & -\gamma \bar{G} D \end{bmatrix},$$

and e_0^T is the row vector $(1, 0, \ldots, 0)$ of length $M + 1$ (retained from $A^{(2)}$), and the J_k are $M \times (M + 1)$ matrices $\bar{G}\partial S/\partial v$ with v being x_1, x_2, or w. If $A^{(3)}$ is nonsingular, then this system has index 0 and the original system (on which two differentiation/rearrangement operations have been done) has index 2. If $A^{(3)}$ is singular, the original index is ≥ 3.

Clearly row operations in $A^{(3)}$ can be done to eliminate the blocks $G - N_2$, N_1, J_1, J_2, J_3 by use of the top three block-rows. Thus the question of singularity of $A^{(3)}$ is equivalent to that of

$$B^{(3)} = \begin{bmatrix} E_2 + I_0 & -E_1 \\ 0 & e_0^T \\ -\gamma \bar{G} D & -\gamma \bar{G} D \end{bmatrix},$$

a square matrix of order $2(M + 1)$. Without affecting the singularity of $B^{(3)}$, we may do elementary column operations on it. Specifically, subtracting the right block-column from the left one gives a matrix

$$B^{(4)} = \begin{bmatrix} E_1 + E_2 + I_0 & -E_1 \\ -e_0^T & e_0^T \\ 0 & -\gamma \bar{G} D \end{bmatrix}.$$

Since $E_1 + E_2 + I_0 = \text{diag}(1, x_1^1 + x_2^1, \ldots, x_1^M + x_2^M)$, we may use row 0 to eliminate the entry $-e_0^T$ in $B^{(4)}$, giving

$$B^{(5)} = \begin{bmatrix} E_1 + E_2 + I_0 & -E_1 \\ 0 & e_0^T \\ 0 & -\gamma \bar{G} D \end{bmatrix}.$$

The singularity of $B^{(5)}$ is equivalent to that of the lower right block

$$B^{(6)} = \begin{bmatrix} e_0^T \\ \\ -\gamma \bar{G} D \end{bmatrix},$$

of order $M+1$. Row 0 in $B^{(6)}$ can be used to eliminate column 0 of the rest, leaving

$$B^{(7)} = \begin{bmatrix} 1 & 0 \\ \\ 0 & -\gamma \bar{G} \bar{D} \end{bmatrix},$$

where $\bar{D}$ is D with column 0 removed. Thus the singularity of $B^{(7)}$ is equivalent to that of the $M \times M$ matrix $\bar{G}\bar{D}$.

Proving that $\bar{G}\bar{D}$ is nonsingular appears to require using detailed information about $\bar{G}$ and $\bar{D}$. We have proven the result only for one particular choice, which is based on 3-point differences. Specifically, the discrete gradient $\bar{G}z = x$ can be described in terms of

$$\left.\begin{aligned} \delta_j &= \eta_j - \eta_{j-1} \\ s^j &= (z^j - z^{j-1})/\delta_j \qquad (1 \le j \le M) \end{aligned}\right\} \tag{2.6}$$

by the relations

$$\left.\begin{aligned} x^1 &= (\delta_2 s^1 + \delta_1 s^2)/(\delta_1 + \delta_2) \\ &\cdots \\ x^j &= (\delta_{j+1} s^j + \delta_j s^{j+1})/(\delta_j + \delta_{j+1}) \qquad (1 \le j \le M-1) \\ &\cdots \\ x^M &= -Sh\, z^M. \end{aligned}\right\} \tag{2.7}$$

The discrete divergence $\bar{D}u = z$ is based on a three-point difference approximation to the continuous derivative $3\partial\left(\eta^2 u(\eta)\right)/\partial(\eta^3)$, with a two point approximation at each boundary. Thus we define

$$v^j = \eta_j^2 u^j \qquad (1 \le j \le M) \tag{2.8a}$$

and

$$\epsilon_j = \eta_j^3 - \eta_{j-1}^3 \qquad (1 \le j \le M) \tag{2.8b}$$

and the two-point difference quotients

$$\left.\begin{aligned} w^1 &= 3v^1/\epsilon_1 \\ w^2 &= 3(v^2 - v^1)/\epsilon_2 \\ &\cdots \\ w^j &= 3(v^j - v^{j-1})/\epsilon_j \qquad (2 \le j \le M). \end{aligned}\right\} \tag{2.8c}$$

Then $z = \bar{D}u$ is defined by

$$\left.\begin{array}{rcll} z^0 &=& w^1 & \\ z^1 &=& \frac{\epsilon_1}{\epsilon_2+\epsilon_1}w^2 + \frac{\epsilon_2}{\epsilon_2+\epsilon_1}w^1 & \\ \cdots & & & \\ z^j &=& \frac{\epsilon_j}{\epsilon_{j+1}+\epsilon_j}w^{j+1} + \frac{\epsilon_{j+1}}{\epsilon_{j+1}+\epsilon_j}w^j & (1 \le j \le M-1) \\ \cdots & & & \\ z^M &=& w^M. & \end{array}\right\} \quad (2.8d)$$

We can now prove the desired result.

Theorem 2.1. *With the definitions (2.6)–(2.8) for the discrete gradient $\bar{G}$ and discrete divergence $\bar{D}$, the $M \times M$ matrix $\bar{G}\bar{D}$ is nonsingular.*

Proof: Suppose there is a vector u with $\bar{D}u = z$ and $\bar{G}z = 0$. We must show that $u = 0$. From (2.7) for $\bar{G}z = x$ with $x = 0$, we get, in terms of the s^j of (2.6),

$$\begin{array}{rcll} z^M &=& 0 \quad \text{and} & \\ s^{j+1} &=& -(\delta_{j+1}/\delta_j)s^j & (1 \le j \le M-1). \end{array} \quad (2.9)$$

Defining new quantities

$$t^j = s^j/\delta_j = (z^j - z^{j-1})/\delta_j^2 \qquad (1 \le j \le M), \quad (2.10)$$

the result (2.9) gives

$$t^j = (-1)^{j-1}t^1 \qquad (1 \le j \le M). \quad (2.11)$$

Together with $z^M = 0$ and the definition (2.10), the result (2.11) says that each z^j is proportional to t^1, or that the null space of $\bar{G}$ in $(M+1)$-space is one-dimensional.

Next, we use the equations (2.8) defining $z = \bar{D}u$. Rewrite (2.8d) as

$$\left.\begin{array}{rcll} z^0 &=& w^1 & \\ (\epsilon_2+\epsilon_1)z^1 &=& \epsilon_1 w^2 + \epsilon_2 w^1 & \\ \cdots & & & \\ (\epsilon_{j+1}+\epsilon_j)z^j &=& \epsilon_j w^{j+1} + \epsilon_{j+1}w^j & (1 \le j \le M-1) \\ \cdots & & & \\ z^M &=& w^M. & \end{array}\right\} \quad (2.12)$$

In these equations, perform operations to eliminate $w^1, w^2, \ldots, w^M$ in turn, starting with

$$(\epsilon_2+\epsilon_1)z^1 - \epsilon_2 z^0 = \epsilon_1 z^1 + \epsilon_2(z^1 - z^0) = \epsilon_1 w^2.$$

Subtract ϵ_3 times this equation from the equation for z^2, multiplied by ϵ_1, to get

$$\epsilon_1\epsilon_2 z^2 + \epsilon_1\epsilon_3(z^2 - z^1) - \epsilon_2\epsilon_3(z^1 - z^0) = \epsilon_1\epsilon_2 w^3.$$

Continuing, having an equation with $\epsilon_1 \ldots \epsilon_{j-1} w^j$ on the right, subtract ϵ_{j+1} times this equation from the equation in (2.12) for z^j, multiplied by $\epsilon_1\epsilon_2 \ldots \epsilon_{j-1}$, to get

$$\left(\prod_1^j \epsilon_i\right) z^j + \left(\prod_1^{j+1} \epsilon_i\right) [\,(z^j - z^{j-1})/\epsilon_j - (z^{j-1} - z^{j-2})/\epsilon_{j-1} + \ldots + (-1)^{j-1}(z^1 - z^0)/\epsilon_1\,]$$
$$= \left(\prod_1^j \epsilon_i\right) w^{j+1} \qquad (2.13)$$

for $j = 1, 2, \ldots, M-1$. This can easily be proved rigorously by induction. Finally, taking (2.13) for $j = M-1$ and applying the above operation one more time, using $\epsilon_M z^M = \epsilon_M w^M$ from (2.12),

$$\left(\prod_1^M \epsilon_i\right) \left[(z^M - z^{M-1})/\epsilon_M - (z^{M-1} - z^{M-2})/\epsilon_{M-1} + \ldots + (-1)^{M-1}(z^1 - z^0)/\epsilon_1\right] = 0\,.$$

Substitution from (2.10) and (2.11) and division by $\epsilon_1\epsilon_2 \ldots \epsilon_M$ gives

$$(-1)^{M-1} t^1 \delta_M^2/\epsilon_M + (-1)^{M-1} t^1 \delta_{M-1}^2/\epsilon_{M-1} + \ldots + (-1)^{M-1} t^1 \delta_1^2/\epsilon_1 = 0,$$

in which the alternating signs have all become the same, owing to (2.11). But in this equation the coefficient of $(-1)^{M-1} t^1$ is

$$\sum_1^M \delta_j^2/\epsilon_j > 0,$$

and so we conclude that $t^1 = 0$ and hence all $t^j = 0$. By (2.10), this in turn implies $z^j - z^{j-1} = 0$ for $j = 1, \ldots, M$, or $z^0 = z^1 = \ldots = z^M = 0$. Now the relations between u, v, w, and z are invertible, so that $z = 0$ implies $w = 0$ from (2.12), which implies $v = 0$ from (2.8c), and finally $u = 0$. **Q.E.D.**

We have therefore proved, at least for the particular discretizations used, that the matrices GD, $B^{(7)}$, $\ldots$, $B^{(3)}$, and $A^{(3)}$ are all nonsingular, and hence that *the original DAE system (2.1) has index 2.* The result is probably true for more general choices of discretizations as well.

The sequence of operations proving that the index of (2.1) is 2 also proves that it is consistent and solvable, provided that consistent initial conditions are imposed, and that the solution is unique for given consistent initial conditions. These results follow from an examination of the sequence of systems (2.2), (2.3), (2.4), (2.5) in reverse order, as follows.

First, the nonsingularity of $A^{(3)}$ means that the system (2.5) has index 0, and is uniquely solvable for any initial y vector y_0 at $t = 0$. The corresponding initial $\dot{y}$ vector is

$$\dot{y}_0 = (A^{(3)})^{-1} g^{(3)}(y_0).$$

Next, recall that (2.5) arose from (2.4) by differentiating the final block of M equations,

$$0 = \bar{G}\left[S_1 + S_2 - \gamma D(n_1 + n_2)\right]. \tag{2.14}$$

Thus the system (2.4) has index 1, and an initial vector y_0 is consistent for (2.4) only if it satisfies the M constraints (2.14). Conversely, for any y_0 satisfying (2.14), (2.4) has a unique solution, which is also the solution of the index 0 system (2.5). The row operations that produced (2.4) from (2.3) are easily reversible and involve no differentiations and so the same solvability statement holds for the index 1 system (2.3). Finally, recall that (2.3) came from (2.2) by differentiation of the $2(M+1)$ equations

$$g_4 = 0, \qquad g_5 = 0. \tag{2.15}$$

Hence y_0 is consistent for (2.2) if and only if it satisfies both (2.14) and (2.15), and in that case the solutions of (2.2), (2.3), (2.4), and (2.5) are identical. That is, the original system, (2.1) or (2.2), is solvable and has a unique solution y for any given initial vector y_0 which satisfies the equations

$$\left.\begin{aligned} I_0 n_1 + E_2 n_1 - E_1 n_2 + G x_1 + b_1 &= 0 \\ I_0 n_2 + E_1 n_2 - E_2 n_1 + G x_2 + b_2 &= 0 \\ \bar{G}\left[S_1 + S_2 - \gamma D(n_1 + n_2)\right] &= 0 \end{aligned}\right\} \tag{2.16}$$

which are both necessary and sufficient conditions on y_0 for the existence of a solution. Note that the first two equations in (2.16) are just the discretized Stefan-Maxwell equations, combined with the equations $n_1^0 = n_2^0 = 0$.

3 Fluid Conservation in the Initial Model

The original model (2.1) is well-posed and has index 2. But an issue of equal importance is whether the conservation relation

$$x_1^j + x_2^j = 1 \tag{3.1}$$

holds for the discrete DAE system, as it is known to for the original continuous problem.

We will examine this question by using an equivalent reformulation of the problem, in which the deviations from (3.1) occur explicitly. Thus define a vector of unit components

$$u = (1, \ldots, 1)^T \qquad (\text{length } M + 1),$$

and a new dependent variable vector (the deviations)

$$z = x_1 + x_2 - u. \tag{3.2}$$

We will change variables from x_1 and x_2 to x_1 and z. Similarly, in view of the way the fluxes n_k enter into the model, it is convenient to define the vector of discrete total fluxes

$$n = n_1 + n_2. \tag{3.3}$$

We will change variables from n_1 and n_2 to n_1 and n, using the sum of the two original flux equations in place of the last equation.

Specifically, the system in terms of $(x_1, z, w, n_1, n)^T$, using (2.1), is

$$\left.\begin{aligned}
\dot{x}_1 &= S_1 - \gamma D n_1 \\
\dot{z} &= g_1 + g_2 = S - \gamma D n \\
\dot{w} &= S_3 \\
0 &= I_0 n_1 + E_2 n_1 - E_1(n - n_1) + G x_1 + b_1 \\
0 &= g_4 + g_5 = I_0 n + G(z + u) + b_1 + b_2.
\end{aligned}\right\} \tag{3.4}$$

Note that the matrix coefficient of n_1 above is

$$I_0 + E_1 + E_2 = \operatorname{diag}(1, x_1^1 + x_2^1, \ldots, x_1^M + x_2^M)$$

$$= I + \text{diag}\,(0,\, z^1,\, \ldots,\, z^M)$$

$$= I + Z,$$

defining $Z = \text{diag}\,(0, z^1, \ldots, z^M)$. Also, the discrete gradient G produces a zero result from the vector u of constants, except at the boundary, so that

$$Gu = (0, 0, \ldots, 0, -Sh)^T.$$

Since

$$b_1 + b_2 = (0, 0, \ldots, 0, Sh(x_{1b} + x_{2b}))^T$$

with $x_{1b} + x_{2b} = 1$, we get

$$Gu + b_1 + b_2 = 0.$$

Thus (3.4) simplifies to

$$\left.\begin{aligned} \dot{x}_1 &= S_1 - \gamma D n_1 \\ \dot{z} &= S - \gamma D n \\ \dot{w} &= S_3 \\ 0 &= n_1 + Z n_1 - E_1 n + G x_1 + b_1 \\ 0 &= I_0 n + G z. \end{aligned}\right\} \tag{3.5}$$

Next we perform a reduction process on this system analogous to that in Section 2, in order to determine whether $z = 0$ in the solution, provided that $z = 0$ initially. First, differentiating the algebraic part of (3.5), we get

$$\left.\begin{aligned} (G - N)\dot{x}_1 + N_1 \dot{z} + (I + Z)\dot{n}_1 - E_1 \dot{n} &= 0 \\ G\dot{z} + I_0 \dot{n} &= 0, \end{aligned}\right\} \tag{3.6}$$

where we have defined

$$N = N_1 + N_2 = \text{diag}\,(0, n^1, \ldots, n^M).$$

Elimination of $\dot{x}_1$ and $\dot{z}$ from (3.6) using the differential part of (3.5) gives

$$\left.\begin{aligned} (I + Z)\dot{n}_1 - E_1 \dot{n} &= (N - G)(S_1 - \gamma D n_1) - N_1(S - \gamma D n) \\ I_0 \dot{n} &= -G(S - \gamma D n). \end{aligned}\right\} \tag{3.7}$$

As shown earlier, the square matrix multiplying $(\dot{n}_1, \dot{n})^T$ in (3.7) has rank $M+2$, leaving the last M equations as algebraic. With a sign change, this algebraic system is

$$0 = \bar{G}(S - \gamma D n). \qquad (3.8)$$

Consider a solution of the system (3.5), as generated from consistent initial conditions that satisfy $z = 0$, the algebraic part of (3.5), and (3.8). We have shown that this initial value problem is solvable, and has a unique solution. Thus to determine whether or not $z \equiv 0$ in that solution we need only see whether the system with z and $\dot{z}$ eliminated is also solvable. That is, if the system

$$\left.\begin{aligned} \dot{x}_1 &= S_1 - \gamma D n_1 \\ \dot{w} &= S_3 \\ 0 &= S - \gamma D n \\ 0 &= n_1 - E_1 n + G x_1 + b_1 \\ 0 &= I_0 n \end{aligned}\right\} \qquad (3.9)$$

is solvable for any given initial conditions satisfying the algebraic part of (3.9) and (3.8), then the solution, augmented by $z \equiv 0$, must be the unique solution of (3.5).

Consider the problem of choosing initial values for n_1 and n consistent with (3.9), given an initial x_1 and w. The algebraic part of (3.9) is equivalent to the equations

$$n_1^0 = 0, \qquad n^0 = 0 \qquad (3.10a)$$

$$x_1^j n^j - n_1^j = (G x_1 + b_1)_j \qquad (j = 1, \ldots, M) \qquad (3.10b)$$

$$D n = \gamma^{-1} S \qquad (3.10c)$$

On eliminating n_1^0 and n^0 by (3.10a), we have $2M+1$ equations (3.10b) and (3.10c) in the $2M$ unknowns n_1^j, n^j $(j = 1, \ldots, M)$. If we denote by $\hat{D}$ the matrix D with row 0 and column 0 removed, and denote by $\hat{S}$, $\hat{n}_1$, $\hat{n}$ the vectors S, n_1, n with component 0 removed, then (3.10c) is equivalent to

$$\hat{D}\hat{n} = \gamma^{-1}\hat{S} \qquad (3.11)$$

and

$$\sum_{j=1}^{M} d_{0j} n^j = \gamma^{-1} S^0. \tag{3.12}$$

We next observe that the $M \times M$ matrix $\hat{D}$ is nonsingular, at least for the particular discretization used here.

Theorem 3.1. *With the definition of discrete divergence D given by (2.8), the $M \times M$ matrix $\hat{D}$, gotten from D by removing row and column 0, is nonsingular.*

Proof: Given a vector $u = (u^1, \ldots, u^M)^T$, and defining $v^j = \eta_j^2 u^j$, $\epsilon_j = \eta_j^3 - \eta_{j-1}^3$, and $w^j = 3(v^j - v^{j-1})/\epsilon_j$ $(w^1 = 3v^1/\epsilon_1)$ as in (2.8), the components of $\hat{D}u$ are given by (2.8d) with the equation $z^0 = w^1$ removed. If $\hat{D}u = 0$, then $z^M = 0$, $z^{M-1} = 0$, $\ldots$ in turn imply $w^M = 0$, $w^{M-1} = 0$, $\ldots$, $w^1 = 0$. But from (2.8c) this implies $v^1 = v^2 = \ldots = v^M = 0$, and hence $u = 0$. It follows that $\hat{D}$ is nonsingular. **Q.E.D.**

Now (3.11) allows us to express $\hat{n} = (n^1, \ldots, n^M)^T$ in terms of the given x_1 and w, namely as $\hat{n} = \gamma^{-1}\hat{D}^{-1}\hat{S}$. But then (3.12) requires this vector to satisfy

$$S^0 = \sum_{j=1}^{M} d_{0j}\gamma n^j = \sum_{j=1}^{M} d_{0j}(\hat{D}^{-1}\hat{S})_j. \tag{3.13}$$

This is a relation that involves only the initial values of x_1 and w (and $x_2 = 1 - x_1$) by way of the total fluid source function $S = S_1 + S_2$. In general, this relation will *not* hold.

To take a specific example, consider the case $M = 2$, for which (using (2.8))

$$D = \begin{pmatrix} 0 & 3/\eta_1 & 0 \\ 0 & (\hat{D}) & \\ 0 & & \end{pmatrix}$$

with

$$\hat{D} = \frac{3}{1-\eta_1^3} \begin{pmatrix} \frac{1-2\eta_1^3}{\eta_1} & \eta_1^3 \\ \eta_1^2 & 1 \end{pmatrix}.$$

Given $S = (S^0, S^1, S^2)^T$, we find

$$\gamma \begin{pmatrix} n^1 \\ n^2 \end{pmatrix} = \hat{D}^{-1}\hat{S} = \frac{1}{3(1-\eta_1^3)} \begin{pmatrix} \eta_1(S^1 - n_1^3 S^2) \\ \eta_1^3 S^1 + (1 - 2n_1^3)S^2 \end{pmatrix}$$

so that (3.13) becomes

$$S^0 = \frac{S^1 - \eta_1^3 S^2}{1 - \eta_1^3}, \quad \text{or}$$

$$S^1 = (1 - \eta_1^3)S^0 + \eta_1^3 S^2. \tag{3.14}$$

This requires S^1 to be a certain weighted average of S^0 and S^2. Clearly, for an arbitrary choice of the initial x_1 and w, (3.14) can fail to hold. In the special case (which corresponds to the actual initialization used) where the initial profiles are taken to be flat, we will have $S^0 = S^1 = S^2$, and then (3.14) does hold. However, the profiles deviate from flatness immediately and (3.14) will then fail.

Although all of the above discussion is phrased in terms of consistency of *initial* conditions, it applies equally well to any time point. Thus at any given time t, if we have values of x_1, w, n_1, n consistent with (3.9), then (3.10) holds and x_1 and w must satisfy (3.13). This in general is not true.

4 Adjusting the Initial Model

The absence of guaranteed conservation (3.1) in the discrete form of the original continuous equations (which themselves do guarantee conservation) is disturbing. Since the proof of conservation for the continuous equations works from the surface boundary conditions inwards, it is reasonable to expect that an adjustment of the discrete system at the origin will bring about (3.1). For such an adjustment, we can appeal to the fluxless form of the continuous model. There, the fluid equations at the origin are

$$\left.\begin{aligned} \dot{x}_1^0 &= x_2^0 S_1^0 - x_1^0 S_2^0 + \gamma \nabla^2 x_1^0 \\ \dot{x}_2^0 &= x_1^0 S_2^0 - x_2^0 S_1^0 + \gamma \nabla^2 x_2^0. \end{aligned}\right\} \tag{4.1}$$

The final term in each equation (4.1) is a Laplacian at the origin, for which the appropriate 2-point discrete approximation is

$$\nabla^2 x_i^0 = 6(x_i^1 - x_i^0)/n_1^2. \tag{4.2}$$

To analyze the solvability of this adjusted model, we first represent it in a vector form similar to (2.1), where only the 0th components of g_1 and g_2 are altered. Define D_0 to be the discrete divergence operator D with row 0 replaced by $(0, \ldots, 0)$. Then define vectors of length $M+1$,

$$\left.\begin{aligned} R_1 &= (R_1^0, 0, \ldots, 0)^T \\ R_2 &= (R_2^0, 0, \ldots, 0)^T \\ R_1^0 &= -x_1^0 S_2^0 - (1 - x_2^0) S_1^0 + 6\gamma(x_1^1 - x_1^0)/n_1^2 \\ R_2^0 &= -x_2^0 S_1^0 - (1 - x_1^0) S_2^0 + 6\gamma(x_2^1 - x_2^0)/n_1^2. \end{aligned}\right\} \tag{4.3}$$

Then the adjusted model can be written

$$\left.\begin{aligned} \dot{x}_1 &= S_1 - \gamma D_0 n_1 + R_1 \equiv h_1 \\ \dot{x}_2 &= S_2 - \gamma D_0 n_2 + R_2 \equiv h_2 \\ \dot{w} &= S_3 \equiv h_3 \\ 0 &= I_0 n_1 + E_2 n_1 - E_1 n_2 + G x_1 + b_1 \equiv h_4 \\ 0 &= I_0 n_2 + E_1 n_2 - E_2 n_1 + G x_2 + b_2 \equiv h_5. \end{aligned}\right\} \tag{4.4}$$

Note that h_3, h_4, and h_5 are the same as the g_3, g_4, and g_5 of (2.1). In compact form, this is

$$A\dot{y} = h(y) \tag{4.5}$$

with the same matrix A as in (2.2).

Proceeding as before, we differentiate the algebraic part of (4.5) and manipulate the result so as to maximize the number of zero rows in the matrix multiplying $\dot{y}$. The result will be identical to that for the unaltered model, except in the two equations for $\dot{x}_i^0$. After the same manipulation of the last two block-rows, we get

$$A^{(2)}\dot{y} = h^{(2)} \tag{4.6}$$

with $A^{(2)}$ as in (2.4), and

$$h^{(2)} = (h_1, h_2, h_3, 0, -G(h_1 + h_2))^T.$$

Here $A^{(2)}$ has M zero rows, and that number cannot be increased. Thus the system (4.4) has index ≥ 2, and we proceed to differentiate the algebraic part of (4.6). In terms of the $M \times (M+1)$

matrix $\bar{G}$ (G with row 0 removed), this algebraic system is

$$0 = \bar{G}(h_1 + h_2) = \bar{G}(S - \gamma D_0(n_1 + n_2) + R)$$

where $S = S_1 + S_2$, $R = R_1 + R_2 = (R^0, 0, \ldots, 0)^T$. Note that

$$R^0 = -S^0 + 6\gamma\eta_1^{-2}(x_1^1 + x_2^1 - x_1^0 - x_2^0).$$

In the notation used before, the result of differentiating this equation is

$$0 = J_1\dot{x}_1 + J_2\dot{x}_2 + J_3\dot{w} - \gamma\bar{G}D_0(\dot{n}_1 + \dot{n}_2) + \bar{G}\dot{R}$$

where

$$\begin{aligned} \dot{R} &= (\dot{R}^0, 0, \ldots, 0)^T \\ \dot{R}^0 &= -(\partial S^0/\partial x_1^0)\dot{x}_1^0 - (\partial S^0/\partial x_2^0)\dot{x}_2^0 - (\partial S^0/\partial w^0)\dot{w}^0 + 6\gamma n_1^{-2}(\dot{x}_1^1 + \dot{x}_2^1 - \dot{x}_1^0 - \dot{x}_2^0). \end{aligned}$$

Collecting the coefficients of $\dot{x}_1$, $\dot{x}_2$, and $\dot{w}$, we have a system

$$\bar{A}^{(3)}\dot{y} = h^{(3)} = (h_1, h_2, h_3, 0, 0)^T, \qquad (4.7)$$

where

$$\bar{A}^{(3)} = \begin{bmatrix} I & & & & \\ & I & & & \\ & & I & & \\ G - N_2 & N_1 & 0 & E_2 + I_0 & -E_1 \\ 0 & 0 & 0 & 0 & e_0^T \\ \bar{J}_1 & \bar{J}_2 & \bar{J}_3 & -\gamma\bar{G}D_0 & -\gamma\bar{G}D_0 \end{bmatrix}.$$

The block $\bar{J}_k$ is J_k augmented with coefficients from $\dot{R}^0$. If $\bar{A}^{(3)}$ is nonsingular then (4.7) has index 0 and (4.4) has index 2.

As with $A^{(3)}$ in (2.5), the blocks $G - N_2$, N_1, and the $\bar{J}_k$ can be eliminated in $\bar{A}^{(3)}$, so that we need only examine the square matrix

$$\bar{B}^{(3)} = \begin{bmatrix} E_2 + I_0 & -E_1 \\ 0 & e_0^T \\ -\gamma\bar{G}D_0 & -\gamma\bar{G}D_0 \end{bmatrix}$$

of order $2(M+1)$. Likewise block-column operations give

$$B^{(4)} = \begin{bmatrix} E_1 + E_2 + I_0 & -E_1 \\ -e_0^T & e_0^T \\ 0 & -\gamma\bar{G}D_0 \end{bmatrix},$$

in which the upper left block is nonsingular and the left middle block $-e_0^T$ can be eliminated. This gives a square matrix of order $M+1$,

$$\bar{B}^{(6)} = \begin{bmatrix} e_0^T \\ -\gamma\bar{G}D_0 \end{bmatrix}$$

whose singularity must be determined. Also as before, row 0 of $\bar{B}^{(6)}$ can be used to eliminate column 0 of the rest, leaving

$$\bar{B}^{(7)} = \begin{bmatrix} 1 & 0 \\ 0 & -\gamma\bar{G}\bar{D}_0 \end{bmatrix}$$

where $\bar{D}_0$ is D_0 with column 0 deleted, or $\bar{D}$ with row 0 replaced by zero. The singularity of $\bar{B}^{(7)}$ (hence $\bar{A}^{(3)}$) is equivalent to that of the $M \times M$ matrix $\bar{G}\bar{D}_0$.

To study this matrix, define

$$\hat{G} = (\bar{G} \text{ with column 0 removed}) = (G \text{ with row 0 and column 0 removed})$$

and

$$\hat{D} = (\bar{D}_0 \text{ with row 0 removed}) = (D \text{ with row 0 and column 0 removed}).$$

Then, because $\bar{D}_0$ has only zeros in row 0, we have

$$\bar{G}\bar{D}_0 = \hat{G}\hat{D}, \tag{4.8}$$

the product of two $M \times M$ matrices. For the discrete divergence given by (2.8), the nonsingularity of $\hat{D}$ was proved in the previous section. Thus we need only study the nonsingularity of $\hat{G}$.

Theorem 4.1. *For the discrete gradient defined by (2.6)–(2.7), the matrix $\hat{G}$ is nonsingular provided that*

$$\eta_1^2 - (\eta_2 - \eta_1)^2 + \ldots + (-1)^{M-1}(1 - \eta_{M-1})^2 \neq 0. \tag{4.9}$$

Proof: Equations (2.6)–(2.7) define $x = \bar{G}z$, where $\bar{G}$ is G with row 0 removed. Thus the same equations with z^0 replaced by 0 define $x = \hat{G}z$ for $z = (z^1, \ldots, z^M)^T$. Suppose $x = 0$. Then by (2.7), $z^M = 0$ and

$$\delta_{j+1}s^j + \delta_j s^{j+1} = 0 \qquad (1 \leq j \leq M-1).$$

Thus

$$s^j/\delta_j = (-1)^{j-1}s^1/\delta_1 \qquad (1 \leq j \leq M).$$

From the definitions (2.6), this gives

$$z^j - z^{j-1} = (-1)^{j-1}\delta_j^2 z^1/\delta_1^2 \qquad (2 \leq j \leq M), \tag{4.10}$$

and thus

$$\begin{aligned} z^M &= z^1 + (z^1/\delta_1^2)\sum_{j=2}^{M}(-1)^{j-1}\delta_j^2 \\ &= (z^1/\delta_1^2)\sum_{j=1}^{M}(-1)^{j-1}\delta_j^2. \end{aligned}$$

The last sum above is exactly the left-hand side of (4.9) and so is nonzero by assumption. Thus from $z^M = 0$ we conclude that $z^1 = 0$, and then that all $z^j = 0$ from (4.10), proving that $\hat{G}$ is nonsingular. **Q.E.D.**

The condition (4.9) is essential for this result, and can very well fail to hold. For example, if M is even and the mesh is uniform (the $\delta_j = \eta_j - \eta_{j-1}$ are all equal), the sum in (4.9) vanishes. In what follows, we will assume that the mesh has been picked so that (4.9) does hold. This allows any mesh for which the δ_j are strictly decreasing with j, for then the sum in (4.9) is either

$$(\delta_1^2 - \delta_2^2) + (\delta_3^2 - \delta_4^2) + \ldots + (\delta_{M-1}^2 - \delta_M^2)$$

for M even, or

$$(\delta_1^2 - \delta_2^2) + \ldots + (\delta_{M-2}^2 - \delta_{M-1})^2 + \delta_M^2$$

for M odd, and in either case it is the sum of positive terms. In particular, (4.9) allows the case we most often use in practice, an equal volume mesh, where $\eta_j = (j/M)^{1/3} \quad (0 \le j \le M)$. The concavity of the function $x^{1/3}$ implies that the δ_j are decreasing.

Returning to the relation (4.8), we have established that, for the particular discretizations chosen, the matrix $\bar{G}\bar{D}_0$ is nonsingular, and thus so is the matrix $\bar{A}^{(3)}$ in (4.7). Since the latter is the result of two differentiations on the system (4.4), we have shown that the given model, the initial semi-discrete system with adjustments (4.1) at the origin, *has index 2 and is well-posed.*

To see whether the fluid conservation relation (3.1) holds for this model, we argue as in the previous section. The system (4.4) in x_1, x_2, w, n_1, n_2 is equivalent to a system in x_1, w, n_1, $z = x_1 + x_2 - u$, and $n = n_1 + n_2$, namely

$$\left.\begin{aligned} \dot{x}_1 &= S_1 - \gamma D_0 n_1 + R_1 \\ \dot{z} &= h_1 + h_2 = S - \gamma D_0 n + R \\ \dot{w} &= S_3 \\ 0 &= (I + Z)n_1 - E_1 n + G x_1 + b_1 \\ 0 &= I_0 n + G z \end{aligned}\right\} \qquad (4.11)$$

in analogy with (3.5). This system is uniquely solvable and has index 2. To see whether $z \equiv 0$ in the solution, it is sufficient to see whether the system derived from (4.11) by dropping z and $\dot{z}$ is also uniquely solvable. If so, that solution, augmented by $z \equiv 0$, must also be the solution of (4.11), by uniqueness.

The system corresponding to (4.11) with $z \equiv 0$ is

$$\left.\begin{aligned} \dot{x}_1 &= S_1 - \gamma D_0 n_1 + R_1 \\ \dot{w} &= S_3 \\ 0 &= S + R - \gamma D_0 n \\ 0 &= n_1 - E_1 n + G x_1 + b_1 \\ 0 &= I_0 n. \end{aligned}\right\} \qquad (4.12)$$

Here the 0th components of R_1 and $R = R_1 + R_2$, using $x_1^j + x_2^j = 1$ in (4.3), are

$$R_1^0 = -x_1^0 S^0 + 6\gamma(x_1^1 - x_1^0)/n_1^2$$
$$R^0 = -S^0.$$

Thus the 0th equation in $S + R - \gamma D_0 n = 0$ is trivially satisfied, and the remaining M equations,

$$\gamma \hat{D} \hat{n} = \hat{S}, \tag{4.13}$$

yield $\hat{n} = (n^1, \ldots, n^M)^T$ uniquely in terms of x_1 and w via $\hat{S} = (S^1, \ldots, S^M)^T$. The last block of (4.12) is simply $n^0 = 0$, and so all of n is uniquely determined from x_1 and w. The fourth block in (4.12) then determines

$$n_1 = E_1 n - G x_1 - b_1 \tag{4.14}$$

completely. So n_1 and n can be eliminated from (4.12), giving a well-posed system in x_1 and w alone. This proves that the solution of the system (4.11) satisfies $z = 0$ identically, provided that $z = 0$ initially.

Because (4.11) came from the system (4.4) by a reversible change of variables, we have shown that any solution of (4.4), starting from consistent initial conditions with $x_1^j + x_2^j = 1$, satisfies this conservation relation identically.

The index analysis for (4.4) also dictates the constraints on initial conditions, as does the conservation analysis above. Given initial vectors x_1, x_2, w with $x_1 + x_2 = u$, the system (4.13) together with $n^0 = 0$ determines the initial n, and (4.14) determines n_1 (and hence $n_2 = n - n_1$). The initial time derivatives of n_1 and n_2 are given by equations taken from (4.7), or by differentiated forms of (4.13) and (4.14).

5 The Fluxless Model

The semi-discrete forms of the fluxless model (1.2) differ from the flux models in two important ways. One is the presence of a discrete Laplacian operator (on the x_k). The other is the use of a discrete divergence (on ν) which is a two-point difference representing midpoint values, rather than a three-point difference representing mesh-point values. The latter alteration is dictated by the need to invert the discrete divergence operator for the vector ν.

On a mesh with M intervals, the discrete vector $\nu = (\nu^0, \ldots, \nu^M)^T$ has components associated with mesh points η_j (as with x_1, x_2, and w). But here the discrete divergence of ν, denoted $T\nu$, is given by

$$\left.\begin{aligned} T\nu &= (t^{1/2}, t^{3/2}, \ldots, t^{M-1/2})^T, \\ t^{j-1/2} &= 3\frac{\eta_j^2\nu^j - \eta_{j-1}^2\nu^{j-1}}{\eta_j^3 - \eta_{j-1}^3} \qquad (j = 1, \ldots, M). \end{aligned}\right\} \tag{5.1}$$

That is, $t^{j-1/2}$ is the natural two-point approximation to $3\partial(\eta^2\nu)/\partial(\eta^3)$ at the midpoint

$$\eta_{j-1/2} = (\eta_{j-1} + \eta_j)/2.$$

To represent the right-hand side of the equation for ν, we define an averaging operator on vectors $f = (f^0, \ldots, f^M)^T$,

$$\left.\begin{aligned} Kf &= (k^{1/2}, \ldots, k^{M-1/2})^T, \\ k^{j-1/2} &= (f^{j-1} + f^j)/2 \qquad (j = 1, \ldots, M). \end{aligned}\right\} \tag{5.2}$$

Thus T and K are bi-diagonal $M \times (M+1)$ matrices. The discrete form of the equation γ div $(\nu \underline{r}) = S = S_1 + S_2$ in the fluxless model is then

$$\gamma T\nu = KS. \tag{5.3}$$

The Laplacian of a function $x(\eta)$ with spherical symmetry is given by

$$\nabla^2 x = \partial^2 x/\partial\eta^2 + (2/\eta)\partial x/\partial\eta. \tag{5.4}$$

In the discretization of (5.4), where $x(\eta)$ becomes a vector $x = (x^0, \ldots, x^M)^T$, we use three-point formulas for the two derivatives, with appropriate two-point expressions at the boundaries. At the outer boundary, we invoke the boundary condition, which has the form

$$x_\eta = Sh(x_b - x) \qquad \text{at } \eta = 1,$$

in terms of the bulk value x_b. As a result, the discrete Laplacian of x at η_j is a linear homogeneous expression in x except for $j = M$ where there is an inhomogeneous term

$$\left(\frac{1}{1-\eta_{M-1/2}}+2\right) Shx_b = 2(1+1/\delta_M)Shx_b.$$

Thus we define vectors $c_k = 2(1+1/\delta_M)b_k \quad (k = 1, 2)$ of length $M+1$, which are zero except for a last component of $2(1+1/\delta_M)Shx_{kb}$. Then, denoting the coefficients of the homogeneous terms by a square matrix L of order $M+1$, the discrete Laplacian of x_k can be written $Lx_k + c_k$.

As before, we denote by Gx the homogeneous part of the discrete gradient. Also, to facilitate the representation of the fluid equations, we define

$$N = \text{diag}\,(\nu^0, \ldots, \nu^M) \qquad \text{and} \qquad X_k = \text{diag}\,(x_k^0, \ldots, x_k^M).$$

The initial form of the discretized fluxless model can therefore be written

$$\left.\begin{array}{rcl} \dot{x}_1 & = & S_1 - X_1 S - \gamma N(Gx_1 + b_1) + \gamma(Lx_1 + c_1) \\ \dot{x}_2 & = & S_2 - X_2 S - \gamma N(Gx_2 + b_2) + \gamma(Lx_2 + c_2) \\ \dot{w} & = & S_3 \\ 0 & = & \nu^0 \\ 0 & = & \gamma T\nu - KS. \end{array}\right\} \tag{5.5}$$

As a DAE system in

$$y = (x_1, x_2, w, \nu)^T,$$

it has index 1. This follows by noting that the algebraic equations in (5.5) uniquely determine ν from S (hence from x_1, x_2, w); the relations (5.1) are easily solved for $\nu^1, \ldots, \nu^M$, given the $t^{j-1/2}$ and using $\nu^0 = 0$.

An equivalent index 0 problem can be formed by posing only the ODEs in (5.5) and incorporating the solution for ν in terms of (x_1, x_2, w) in the evaluation of the right-hand sides of the ODEs.

The issue of conservation in either of these models can be addressed as before. We consider an equivalent system in terms of x_1, w, ν, and

$$z = x_1 + x_2 - u$$

in place of x_2, where $u = (1, \ldots, 1)^T$. The equation for z is the sum of those for x_1 and x_2. Noting that $Gu + b_1 + b_2 = 0$ and $Lu + c_1 + c_2 = 0$, the equivalent system is

$$\left.\begin{aligned} \dot{x}_1 &= S_1 - X_1 S - \gamma N(Gx_1 + b_1) + \gamma(Lx_1 + c_1) \\ \dot{z} &= -ZS - \gamma NGz + \gamma Lz \\ \dot{w} &= S_3 \\ 0 &= \nu^0 \\ 0 &= \gamma T\nu - KS, \end{aligned}\right\} \tag{5.6}$$

where we have defined $Z = \text{diag}\,(z^0, \ldots, z^M)$. For the well-posed index 1 system (5.6), with consistent initial conditions satisfying $z = 0$, the solution satisfies $z = 0$ identically if the system derived from (5.6) with z and $\dot{z}$ removed is solvable. This derived system is

$$\left.\begin{aligned} \dot{x}_1 &= S_1 - X_1 S - \gamma N(Gx_1 + b_1) + \gamma(Lx_1 + c_1) \\ \dot{w} &= S_3 \\ 0 &= \nu^0 \\ 0 &= \gamma T\nu - KS, \end{aligned}\right\} \tag{5.7}$$

with x_2 replaced by $u - x_1$ wherever it occurs. But (5.7) is clearly a well-posed, solvable, index 1 system in (x_1, w, ν) by the same reasoning applied to (5.5). Thus its solution, augmented by $z = 0$, must be the unique solution of (5.6). This shows that the discrete fluxless models satisfy the conservation relations $x_1^j + x_2^j = 1$ as they stand.

The choice of consistent initial values is also much more straightforward with the fluxless models. Given initial profiles for x_1, x_2, and w (such as flat profiles), we simply invert the relations $\gamma T\nu = KS$ for the ν^j, starting from $\nu^0 = 0$. This solution procedure represents a discrete form of the integral

$$\gamma\nu = \eta^{-2} \int_0^{\eta} \xi^2 S(\xi) d\xi. \tag{5.8}$$

But it is crucial to use a discretization here that is completely consistent with the algebraic system $\nu^0 = 0$, $\gamma T\nu = KS$, and not some other quadrature for (5.8). Otherwise, the integration of the DAE system (5.5) would begin with nonzero residuals, from which it may never recover.

References

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