Bounds for systems of coupled advection-diffusion equations with application to the Poisson-Nernst-Plank equations

Jonathan J. Wylie[*]
Department of Mathematics, City University of Hong Kong, Tat Chee Avenue, Hong Kong

B. H. Bradshaw-Hajek[†]
UniSA STEM, University of South Australia, Mawson Lakes, SA, 5095, Australia

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We consider coupled systems of advection-diffusion equations with initial and boundary conditions and determine conditions on the advection terms that allow us to obtain solutions that can be explicitly bounded above and below using the initial and boundary conditions. Given the advection terms, using our methodology one can easily check if such bounds can be obtained and then one can construct the necessary nonlinear transformation to allow the bounds to be determined. We apply this technique to determine bounding quantities for a number of examples. In particular, we show that the three-ion electroneutral Poisson-Nernst-Planck system of equations can be transformed into a system, which allows for the use of our techniques and we determine the bounding quantities. In addition, we determine the general form of advection terms that allow these techniques to be applied and show that our method can be applied to a very wide class of advection-diffusion equations.

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I. INTRODUCTION

In this paper we will consider systems of partial differential equations of the form

$$u_t = u_{xx} + [R(u, v)]_x, \tag{1}$$

$$v_t = v_{xx} + [Q(u, v)]_x, \tag{2}$$

where $R(u, v)$ and $Q(u, v)$ are at least once differentiable. We will derive conditions on $R(u, v)$ and $Q(u, v)$ that allow us to obtain solutions that can be explicitly bounded above and below. We will focus on advection-diffusion systems in one spatial dimension. However, the results presented here can be readily extended to higher dimensions as discussed in the final section.

Equations of this type are fundamental in describing physical phenomena in which two species diffuse while experiencing advection. A notable example is a model for the densities of two different particle types in a bidisperse suspension. This model was originally derived by Esipov [1] and has been subsequently studied by others [2–5]. Another important example is the Poisson-Nernst-Planck (PNP) system of equations that describes the dynamics of electrical charges [6–14]. We will show that the electroneutral PNP equations can be transformed into a format in which the theory we develop may be applied.

Due to its simplicity and utility, the maximum principle has become one of the most useful, well-known, and important tools in analyzing elliptic and parabolic partial differential equations (PDEs) and is now regarded as an essential tool. Maximum principles allow one to obtain important quantitative information about solutions of PDEs. In particular, they can be used to derive bounds, to obtain results about uniqueness, and provide necessary conditions for solvability. Although the theory of maximum principles for a single PDE is relatively well developed, there has been significantly less work on determining such principles for systems of PDEs such as (1) and (2). In this paper, we will show that a broad class of equations of the form (1) and (2) admit a maximum principle and we describe explicit techniques to determine the quantities that obey the maximum principles.

In terms of applications, there are a number of reasons that maximum principles are useful for equations used to model physical phenomena. First, systems often require that the quantities remain within certain bounds. For example, if the PNP equations are used to model ion transport in biological cells, then the healthy operation of the cell typically can only occur for ion concentrations within given ranges [15,16]. If one can determine theoretical bounds for the ranges of concentrations that can occur based on the initial and boundary conditions, then one can derive explicit criteria for maintaining safe concentration levels. Second, the validity of models often depends on certain assumptions. For example, the simplest form of the PNP equations assumes that the ionic concentrations are sufficiently low that steric effects are negligible [17]. Similarly, the equations for suspensions often assume that the particles are sufficiently dilute [18,19]. In such cases, maximum principles can help us to be certain that the solutions we obtain from the equations do not invalidate the assumptions under which the equations were derived. Third, when introducing new models, one may be unsure about issues of uniqueness, possible singularities, or other

[*]mawylie@cityu.edu.hk
[†]bronwyn.hajek@unisa.edu.au

fundamental problems that the model may exhibit. Maximum principles can be extremely useful in determining important theoretical properties of equations and thereby providing a stronger foundation for new model equations [20].

As mentioned above, in this paper we will derive results that are applicable to the PNP equations. The original motivation for PNP was from solid-state electronics and so only included two ion species. For the electroneutral two-ion case, one can readily show that each ion species satisfies a maximum principle [21]. Recently biological applications have become more important and the need to track more than two ion types is critical to a number of phenomena [15,16]. In contrast to the two-ion case, in the case of three-ion species it is easy to see that each ion species does not satisfy a maximum principle. In fact, the three-ion case is significantly more complicated than the two-ion case and even for steady states it is only recently that existence and uniqueness results have been derived [22–24]. Here, in the fully time-dependent three-ion case we will use our theory to derive quantities that satisfy maximum principles and can hence bound the ionic concentrations.

II. BOUNDS FOR SINGLE ADVECTION-DIFFUSION EQUATIONS

We begin by reviewing the basic ideas that underlie the maximum principle arguments for a single advection-diffusion equation

$$u_t = u_{xx} + [S(u)]_x, \tag{3}$$

which can be rewritten in the form

$$u_t = u_{xx} + S'(u)u_x. \tag{4}$$

Here, we assume that $S(u)$ is a differentiable function, and that we have an initial condition, $u_0(x) = u(x, 0)$ that is twice differentiable in space. We also assume a set of boundary conditions prescribed at the edges of the spatial domain, $x = 0$ and $x = \ell$, that are differentiable in time.

In the case where $S(u) = \text{const.}$ (the linear heat equation), the maximum principle is well known (see, for example, Ref. [20]). It states that on a bounded domain, $u(x,t)$ cannot have a (local) maximum at any interior point in the space-time domain. That is, in the space-time domain $D = \{0 \leqslant x \leqslant \ell, 0 \leqslant t \leqslant T\}$, the maximum value of $u(x,t)$ will occur either initially ($t = 0$) or on the sides ($x = 0$ or $x = \ell$). The proof is relatively straightforward, although care must be taken with the technical details to prove that the maximum cannot occur at $t = T$ (except if $x = 0$ or $x = \ell$, or if $u \equiv \text{const.}$).

A number of theoretical results have been derived that ensure existence and uniqueness for single advection-diffusion equations [that is, when $S(u)$ is not constant]. The case of linear advection-diffusion equations has been widely studied and the existence and uniqueness can be guaranteed as long as the coefficients of the derivative terms are bounded. A nice summary of these results can be found in the book by Protter and Weinberger [20]; here we provide a brief overview and refer the reader to the text for more detail.

Intuitively and simply, the maximum principle for advection-diffusion equations may be understood in the following way. Suppose that a maximum occurs at a point (x_0, t_0) that is in the interior of the space-time domain. Since this point is a local maximum it must satisfy $u_t = u_x = 0$ and $u_{xx} \leqslant 0$ at (x_0, t_0). If $u_{xx} < 0$, then evaluation of (4) at (x_0, t_0) leads to an immediate contradiction since the left-hand side is zero while the right-hand side is negative. Hence, a maximum cannot occur in the interior of the space-time domain if $u_{xx} < 0$ there. As a consequence, the maximum must occur on the boundary of the space-time domain, where it is not necessary that both u_t and u_x vanish. We note that in the nongeneric case in which $u_{xx} = 0$ the result also holds. The proof requires a straightforward, but slightly more careful argument that we will not provide here; see, for example, Ref. [20] for details. The only situation that violates the maximum principle is when $u \equiv \text{const.}$, in which case the maximum is achieved everywhere. An associated minimum principle may be obtained by setting $u = -u$.

Protter and Weinberger also argue that a similar theory can be applied to a broad class of nonlinear advection-diffusion equations as long as the coefficients of the derivative terms in the equation remain bounded, that is, $S'(u)$ must be bounded. Pursuing this further, Guilding [25] considered a wide class of nonlinear advection-diffusion equations and derived very general conditions for existence and uniqueness results that allow for the possibility that the coefficients of the derivative terms oscillate wildly or are unbounded. We also note that it is important to restrict ourselves to the case of finite time. This is because, in the nonlinear case, the gradient of the solution can tend to infinity as time tends to infinity even if the coefficients of the derivative terms remain bounded [26]. Moreover, in the case in which the coefficients of the derivative terms are not bounded, blow up of the solution can occur in finite time [27].

III. MAXIMUM PRINCIPLE FOR SYSTEMS

The main idea explained in this section involves considering the equation satisfied by a general function of the fields u and v in (1) and (2), assuming that the partial derivatives of $R(u, v)$ and $Q(u, v)$ exist. We then consider which types of functions satisfy maximum principles and what conditions on the advection terms are required for this to be the case. We begin by defining a general function $W(U, V)$. We will then define $w(x,t) = W(u(x,t), v(x,t))$ where $u(x,t)$ and $v(x,t)$ are solutions of (1) and (2). A straightforward application of the chain rule and eliminating terms involving time derivatives of u and v using (1) and (2) gives

$$\begin{aligned} w_t &= W_U u_t + W_V v_t, \\ &= W_U u_{xx} + W_V v_{xx} + W_U[R_U u_x + R_V v_x] \\ &\quad + W_V[Q_U u_x + Q_V v_x], \end{aligned} \tag{5}$$

where, in a slight abuse of notation, the advection terms in Eqs. (1) and (2) are written as $R(U, V)$ and $Q(U, V)$. A straightforward application of the chain rule also yields

$$w_x = W_U u_x + W_V v_x, \tag{6}$$

and

$$w_{xx} = W_U u_{xx} + W_V v_{xx} + W_{UU} u_x^2 + 2W_{UV} u_x v_x + W_{VV} v_x^2. \tag{7}$$

We next use (6) and (7) to eliminate v_x from (5) to obtain

$$\begin{aligned} w_t = w_{xx} &+ 2\frac{u_x}{W_V^2}[W_U W_{VV} - W_V W_{UV}]w_x \\ &- \frac{W_{VV}}{W_V^2}w_x^2 + \frac{1}{W_V}[W_U R_V + W_V Q_V]w_x \\ &- \frac{u_x^2}{W_V^2}\left[W_V^2 W_{UU} - 2W_U W_V W_{UV} + W_U^2 W_{VV}\right] \\ &+ \frac{u_x}{W_V}\left[W_U W_V R_U - W_U^2 R_V + W_V^2 Q_U - W_U W_V Q_V\right]. \end{aligned} \quad (8)$$

In what follows, we assume that u_x and W_{VV} are bounded, and W_V is bounded away from zero. In general, we will not be able to apply a maximum principle argument to (8) for the following reason. If we attempt to follow a similar argument that we applied in Sec. II and assume that an internal maximum exists, then we must have $w_t = 0$, $w_x = 0$ and $w_{xx} \leqslant 0$ at the maximum point. Substituting this into (8) does not lead to a contradiction because we cannot control the last two terms involving square brackets on the right-hand side of (8). This is not surprising since, up to this point, we have not placed any restrictions on the function $W(U, V)$. However, if we were able to choose the function $W(U, V)$ such that both of these square brackets are identically zero, then at an internal local maximum with $w_t = 0$, $w_x = 0$, and $w_{xx} < 0$ the left-hand side of (8) would be zero and the right-hand side would be negative. This would contradict the possibility of such a local maximum existing. The nongeneric case in which a maximum exists with $w_{xx} = 0$ can be dealt with using similar techniques to those mentioned in Sec. II.

Hence, if the square brackets on the right-hand side of (8) are identically zero, then the resulting $w = W(U, V)$ would satisfy a maximum principle. We hence need to choose $W(U, V)$ such that

$$W_V^2 W_{UU} - 2W_U W_V W_{UV} + W_U^2 W_{VV} = 0 \quad (9)$$

and

$$W_U W_V R_U - W_U^2 R_V + W_V^2 Q_U - W_U W_V Q_V = 0. \quad (10)$$

We note that (9) and (10) only depend on the function $W(U, V)$ and do not depend on the particular form of the solution $u(x, t)$ and $v(x, t)$.

IV. TEST IF ADVECTION TERMS ARE ADMISSIBLE AND DETERMINATION OF *W*

In this section, we show that one can readily use (9) and (10) to check if a given pair of functions $R(U, V)$ and $Q(U, V)$ have the form such that we can obtain a function $W(U, V)$ that obeys a maximum principle. From (10), we immediately see that

$$-R_V\left(\frac{W_U}{W_V}\right)^2 + (R_U - Q_V)\left(\frac{W_U}{W_V}\right) + Q_U = 0. \quad (11)$$

This is a quadratic in W_U/W_V that can be readily solved to yield

$$\frac{W_U}{W_V} = \frac{R_U - Q_V \pm \sqrt{(R_U - Q_V)^2 + 4R_V Q_U}}{2R_V}. \quad (12)$$

It remains to check if (12) is compatible with (9). At first sight, this appears to be nontrivial. However, we can rewrite (9) into the form

$$\frac{\partial}{\partial U}\left[\frac{W_U}{W_V}\right] - \frac{W_U}{W_V}\frac{\partial}{\partial V}\left[\frac{W_U}{W_V}\right] = 0. \quad (13)$$

Hence, the condition for compatibility is simply given by substituting (12) into (13). If this condition is satisfied then Eqs. (1) and (2) will have a quantity $W(U, V)$ that will satisfy a maximum principle. We note that we want to apply maximum principle arguments to the quantity W and therefore we require it to be real. Moreover, U and V are real-valued quantities since they represent the solutions to (1) and (2). Hence, we require the quantity W_U/W_V to be real. This implies that we should require that the compatibility condition also ensures that the expression in the square root in (12) is non-negative. Hence, we must also require that $(R_U - Q_V)^2 + 4R_V Q_U \geqslant 0$ for the ranges of U and V that we will encounter in the problem.

If this condition is indeed satisfied, then one still needs to obtain the function $W(U, V)$. At first sight, it seems as though the most natural way to do this is by solving the first-order hyperbolic equation given by (12). However, $W(U, V)$ must also satisfy the compatibility condition (13). We note that (13) is a first-order hyperbolic equation for the quantity W_U/W_V. Applying the method of characteristics we obtain

$$\frac{d}{dU}\left[\frac{W_U}{W_V}\right] = \frac{\partial}{\partial U}\left[\frac{W_U}{W_V}\right] + \frac{dV}{dU}\frac{\partial}{\partial V}\left[\frac{W_U}{W_V}\right]. \quad (14)$$

Comparing with (13) we find

$$\frac{d}{dU}\left[\frac{W_U}{W_V}\right] = 0 \quad \text{on} \quad \frac{dV}{dU} = -\frac{W_U}{W_V}. \quad (15)$$

Integrating (15) we obtain

$$\frac{W_U}{W_V} = p, \quad (16)$$

where p is the constant of integration.

By comparing with (12), we see that

$$p = \frac{R_U - Q_V \pm \sqrt{(R_U - Q_V)^2 + 4R_V Q_U}}{2R_V}. \quad (17)$$

In general, when solving a hyperbolic equation of the form (13) it is possible for shock formation to occur and for the solution to become multivalued. However, in our case, the solution we obtain in (16) must necessarily be single valued because we are also requiring that it is compatible with (12). Hence, any compatible solution must remain single valued and hence characteristics cannot cross.

In the general case, the quantity on the right-hand side of (17) will be a nontrivial function of U and V. Since this function must be constant along characteristics, different values of p label different characteristic lines. However, there is a special case in which the right-hand side of (17) is a constant p_0. In this case, the only relevant value of p for this problem will be p_0. We will deal with this special case separately later.

Equation (16) is also a first-order hyperbolic equation that can be written in the form

$$W_U - pW_V = 0. \quad (18)$$

Applying the method of characteristics again we obtain

$$\frac{dW}{dU} = \frac{\partial W}{\partial U} + \frac{dV}{dU}\frac{\partial W}{\partial V}. \tag{19}$$

Comparing with (18) we obtain

$$\frac{dW}{dU} = 0 \quad \text{on} \quad \frac{dV}{dU} = -p. \tag{20}$$

This implies that the function W must be constant along characteristic lines given by $\frac{dV}{dU} = -p$. We note that these characteristic lines are identical to the characteristic lines that we obtained in (15). Therefore we can immediately rule out the possibility of characteristics crossing and the solution becoming multivalued. Since p is also constant along these characteristic lines, we can conclude that W can be an arbitrary function of p,

$$W = \widehat{W}(p) = \widehat{W}\left(\frac{R_U - Q_V \pm \sqrt{(R_U - Q_V)^2 + 4R_V Q_U}}{2R_V}\right), \tag{21}$$

where $\widehat{W}$ is the arbitrary function. This is true as long as the right-hand side of (17) is not a constant.

In the case in which the right-hand side of (17) is a constant $p = p_0$, we can directly solve (18) using characteristics to obtain

$$W = \widehat{W}(V + p_0 U). \tag{22}$$

In general, the function $\widehat{W}$ in (21) or (22) can be chosen arbitrarily. However, it is most natural to choose the simplest form of W so that a maximum principle can be obtained. Therefore, in most cases, it will be most natural to choose $\widehat{W}$ to be the identity function.

In order to determine the bounds on W, one simply needs to find the maximum and minimum values that W takes on the union of the boundary and initial data. To illustrate this we introduce some examples in the following sections.

A. Example 1: Three-ion electroneutral Poisson-Nernst-Planck equations

The Nernst-Planck equations that govern the dynamics of the ionic concentrations for three-ion types are given by

$$c_{it} = [c_{ix} + z_i c_i \phi_x]_x \text{ for } i = 1, 2, 3, \tag{23}$$

where $c_1(x,t)$, $c_2(x,t)$, and $c_3(x,t)$ are the ionic concentrations, z_1, z_2, and z_3 are the valences of the ions and $\phi(x,t)$ is the electric field. The equation of electroneutrality is given by

$$z_1c_1 + z_2c_2 + z_3c_3 = 0. \tag{24}$$

We will restrict our attention to the case of electroneutral boundary conditions. The quantities $c_1(x,t)$, $c_2(x,t)$, and $c_3(x,t)$ represent concentrations and so are necessarily nonnegative.

Before continuing, we note that in the case of two-ionic species, it has been shown that both of the ionic species individually satisfy both maximum and minimum principles [21]. However, the three-ion case is considerably more complicated. In fact it is straightforward to show that each individual ionic species does not satisfy maximum and minimum principles. For example, one can choose the boundary and initial conditions for c_1 to be the same constant everywhere and the boundary and initial conditions for the other two ionic species not to be constant everywhere. If the electric field difference imposed across the boundaries is not always zero then, as time evolves, c_1 will deviate from the constant value that we imposed initially and at the boundaries. This clearly illustrates that c_1 does not satisfy maximum and minimum principles and naturally raises the question of whether it is possible to find alternative bounds. However, we cannot directly use the theory developed in this paper because the three-ion electroneutral PNP equations (23) and (24) are clearly not in the form of (1) and (2). Nevertheless, we will show that after some manipulation we can still apply our theory. We begin by multiplying (23) by z_i, summing over $i = 1, 2, 3$ and using (24) to obtain

$$\left[\left(z_1^2c_1 + z_2^2c_2 + z_3^2c_3\right)\phi_x\right]_x = 0. \tag{25}$$

Integrating (25) over x we obtain

$$\phi_x = \frac{g(t)}{z_1^2c_1 + z_2^2c_2 + z_3^2c_3}, \tag{26}$$

where $g(t)$ is a function that must typically be chosen to satisfy the boundary conditions on the electric field. We can now use (24) to eliminate c_3 from (26), and then eliminate ϕ_x from the first two equations of (23) to obtain

$$c_{1t} = c_{1xx} + \left[\frac{g(t)z_1c_1}{z_1(z_1 - z_3)c_1 + z_2(z_2 - z_3)c_2}\right]_x$$

$$c_{2t} = c_{2xx} + \left[\frac{g(t)z_2c_2}{z_1(z_1 - z_3)c_1 + z_2(z_2 - z_3)c_2}\right]_x$$

These equations are in the same format as (1) and (2) with

$$R(c_1, c_2) = \frac{g(t)z_1c_1}{z_1(z_1 - z_3)c_1 + z_2(z_2 - z_3)c_2} \tag{27}$$

$$Q(c_1, c_2) = \frac{g(t)z_2c_2}{z_1(z_1 - z_3)c_1 + z_2(z_2 - z_3)c_2}. \tag{28}$$

Next we look for a function $W \equiv W(C_1, C_2)$ that satisfies a maximum principle. Substituting (27) and (28) into (12) we obtain

$$\frac{W_{C_1}}{W_{C_2}} = -\frac{C_2}{C_1} \quad \text{or} \quad \frac{z_1 - z_3}{z_2 - z_3}.$$

It is straightforward to check that both of these solutions satisfy the compatibility condition (13). Hence, w_1 and w_2 will satisfy maximum principles if

$$w_1 = \widehat{w}_1\left(\frac{c_2}{c_1}\right) \quad \text{and} \quad w_2 = \widehat{w}_2[(z_1 - z_3)c_1 + (z_2 - z_3)c_2]$$

where $\widehat{w}_1$ and $\widehat{w}_2$ are arbitrary functions. To obtain the simplest possible bounds, we choose the identity functions for $\widehat{w}_1$ and $\widehat{w}_2$ so that

$$w_1 = \frac{c_2}{c_1} \quad \text{and} \quad w_2 = (z_1 - z_3)c_1 + (z_2 - z_3)c_2. \tag{29}$$

To confirm that these two quantities do indeed satisfy maximum principles one can simply use the transformation (29) to eliminate c_1 and c_2 in favour of w_1 and w_2 to obtain

$$w_{1t} = w_{1xx} + 2\left[\frac{w_{1x}}{w_1} + \frac{(z_2 - z_3)w_{2x}}{(z_1 - z_3) + (z_2 - z_3)w_1}\right]w_{1x} + g(t)(z_2 - z_1 w_1)\left[\frac{w_1}{z_1(z_1 - z_3) + z_2(z_2 - z_3)w_1}\right]_x$$

$$w_{2t} = w_{2xx}.$$

In order for the various terms in the above equations to remain bounded we require that w_1 is bounded and that both w_1 and $(z_1 - z_3) + (z_2 - z_3)w_1$ are bounded away from zero. In terms of the original variables these conditions will be satisfied if c_1, c_2, and c_3 are bounded away from zero. We note that $z_1(z_1 - z_3) + z_2(z_2 - z_3)w_1$ can be rewritten in the form $z_1^2 c_1 + z_2^2 c_2 + z_3^2 c_3$ and so it must necessarily be bounded away from zero if c_1, c_2, and c_3 are bounded away from zero.

The equation for w_2 is simply a diffusion equation and therefore clearly satisfies a maximum principle. In fact, this equation could have been obtained directly by summing (23) over $i = 1, 2, 3$ and using (24). That is, upon use of (24), w_2 is simply the sum of all three-ion concentrations, weighted by the valence of ion three. On the other hand, on the right-hand side of the equation for w_1, the two terms involving square brackets will be zero if w_{1x} is zero. Hence we can directly apply our theory and so the equation for w_1 will also satisfy maximum and minimum principles. This property is not at all obvious from the form of (23) and (24). Note that w_1 is the ratio of concentrations of ions two and one. Since both w_1 and w_2 are quantities with physical meaning, it follows that the maximum principle could have direct physical applications.

B. Example 2: Coupled Burgers' equations

We next consider the system derived by Esipov that models bidisperse suspensions [1]. Mathematical aspects of this system have been widely studied in the literature. For example, the dynamics of this system have been studied in Ref. [2] and the exact solutions were considered in Refs. [3–5]. After some simple transformations, the convection terms in the model of Esipov [1] take the form

$$R(u, v) = -u^2 + auv \quad \text{and} \quad Q(u, v) = -v^2 + buv.$$

Substituting these expressions into (12) we obtain

$$\frac{W_U}{W_V} = \frac{1}{2aU}[(a + 2)V - (b + 2)U \pm \sqrt{((a + 2)V - (b + 2)U)^2 + 4abUV}]. \quad (30)$$

In the general case, these expressions do not satisfy the compatibility condition (13). However, in the special case in which $a = b = -1$, the compatibility conditions are both satisfied. This special case has actually been widely studied in literature and a number of results have been obtained. In particular, Soliman [5] carefully analyzed this case and obtained exact solutions. If $a = b = -1$, then (30) becomes

$$\frac{W_U}{W_V} = 1 \quad \text{or} \quad -\frac{V}{U}.$$

Hence, we can determine two quantities w_1 and w_2 that satisfy maximum principles. These are given by

$$w_1 = \frac{v}{u} \quad \text{and} \quad w_2 = u + v,$$

where we have chosen the identity functions for $\widehat{w}_1$ and $\widehat{w}_2$. The equations for w_1 and w_2 are then given by

$$w_{1t} = w_{1xx} + \left[2\frac{w_{2x}}{w_2} - 2\frac{w_{1x}}{1 + w_1} - w_2\right]w_{1x}$$

$$w_{2t} = w_{2xx} - 2w_2 w_{2x}.$$

We note that u and v represent densities, which are necessarily non-negative. So, as long as u is bounded away from zero, w_1 and w_2 will remain bounded and w_2 and $1 + w_1$will be bounded away from zero. Hence, the equations clearly satisfy maximum equalities for w_1 and w_2.

C. Example 3

We next consider the nonlinear coupled system with convection terms given by

$$R(u, v) = uv \quad \text{and} \quad Q(u, v) = u + v^2.$$

Substituting these expressions into (12) we obtain

$$\frac{W_U}{W_V} = \frac{-V \pm \sqrt{V^2 + 4U}}{2U}.$$

It is straightforward to verify that these expressions satisfy the compatibility condition (13). Hence the quantities

$$w_1 = \frac{v + \sqrt{v^2 + 4u}}{u} \quad \text{and} \quad w_2 = \frac{v - \sqrt{v^2 + 4u}}{u}$$

will satisfy maximum principles. Here we have chosen $\widehat{w}_1$ and $\widehat{w}_2$ as twice the identity function. The equations for w_1 and w_2 are then given by

$$w_{1t} = w_{1xx} - 2\left[\frac{w_{1x}}{w_1} + \frac{w_1 w_{2x}}{w_2(w_1 - w_2)} + \frac{(w_1 + 2w_2)}{w_1 w_2}\right]w_{1x}$$

$$w_{2t} = w_{2xx} - 2\left[\frac{w_{2x}}{w_2} + \frac{w_2 w_{1x}}{w_1(w_2 - w_1)} + \frac{(w_2 + 2w_1)}{w_1 w_2}\right]w_{2x}.$$

In this case, we also need to impose initial and boundary conditions to ensure that the terms in the square brackets in the above equations remain bounded. First, we need to assume that u is bounded away from zero to ensure that both w_1 and w_2 remain bounded. Moreover, we will assume that $u > 0$. In this case, w_1 will be positive and bounded away from zero and w_2 will be negative and bounded away from zero. Hence, $w_1 - w_2$ will also be bounded away from zero. Therefore, all of the terms in the square brackets in the above two equations will remain bounded. If the boundary and initial conditions satisfy all of these criteria then the system will satisfy maximum and minimum principles.

V. GENERAL FORM OF ADMISSIBLE ADVECTION TERMS

In this section we obtain the general solution to (9) and (10) to derive the most general form of the types of advection terms R and Q for which our approach allows one to derive maximum principles.

As mentioned above we can use the method of characteristics on (13) to obtain

$$\frac{W_U}{W_V} = p \text{ on lines defined by } \frac{dV}{dU} = -\frac{W_U}{W_V}. \quad (31)$$

This can be solved to give

$$V = -p(\xi)U + \xi, \quad (32)$$

where ξ is the value of V at $U = 0$. Here,

$$p(\xi) = \frac{W_U}{W_V}, \quad (33)$$

which is an arbitrary function that is constant along characteristics and hence can be a function of ξ. In fact, it will prove to be convenient to allow arbitrary translations in U and V in (32) so that we obtain

$$V - V_0 = -p(\xi)(U - U_0) + \xi, \quad (34)$$

where V_0 and U_0 are arbitrary constants.

We further note that (33) can be solved along the same characteristics defined in (31) to obtain

$$W(U, V) = W_0(\xi), \quad (35)$$

where W_0 is an arbitrary function.

We now note that (10) can be written in the form

$$\frac{W_U}{W_V}\left[R_U - \frac{W_U}{W_V}R_V\right] + Q_U - \frac{W_U}{W_V}Q_V = 0. \quad (36)$$

This can also be solved along the same characteristics defined in (31) to obtain

$$p(\xi)R(U, V) + Q(U, V) = F(\xi), \quad (37)$$

where $F(\xi)$ is an arbitrary function of ξ.

Equations (34) and (37) define the relationship between $R(U, V)$ and $Q(U, V)$ that is required for the techniques described in this paper to work. Therefore, given a function $R(U, V)$ one has the freedom to choose two arbitrary functions $p(\xi)$ and $F(\xi)$ (and the constants U_0 and V_0) and obtain the set of possible functions $Q(U, V)$.

Here we give two simple examples. Choosing the constant function $p(\xi) \equiv k$ and $U_0 = V_0 = 0$, we can use (34) to obtain $\xi = V + kU$. In this case we obtain the condition $Q(U, V) = F(V + kU) - kR(U, V)$ where F and R are arbitrary functions. In fact, if this is satisfied one could have immediately noticed that one can take a linear combination of (9) and (10) and see that the quantity $V + kU$ satisfies a maximum principle.

Alternatively, we can choose $p(\xi) = -\xi$, $U_0 = 1 - B$, and $V_0 = -A$ and use (34) to obtain $\xi = (V + A)/(U + B)$, where A and B are arbitrary constants. In this case, we obtain the condition

$$Q(U, V) = F\left(\frac{V + A}{U + B}\right) + \left(\frac{V + A}{U + B}\right)R(U, V).$$

In the above expression, F and R can be arbitrary functions. In this case the quantity $(V + A)/(U + B)$ will satisfy a maximum principle.

VI. SUMMARY AND CONCLUSIONS

In many mathematical models, there is a requirement that the physical quantities being described must stay within certain bounds. For example, there may be a requirement that concentrations remain positive, or that particle densities remain below certain limits. As a consequence of these types of requirements, it is important to understand the conditions that must be satisfied by the model equations in order for specific quantities to satisfy these conditions.

In this paper, we have considered a general system of two advection-diffusion equations and determined conditions on the advection terms that ensure that specific quantities remain within certain bounds. Surprisingly we have shown that this only requires that a function of the original variables, $W(u(x, t), v(x, t))$, can be found that satisfies Eq. (12) and the compatibility condition (13). The simplicity of these conditions is unexpected given that we have considered an arbitrary system of advection-diffusion equations. That is, despite the generality and possible nonlinearity of the advection terms, we can still find specific quantities that remain within explicit bounds. Given that this condition is satisfied, we also explicitly show how to construct the function $W(u, v)$ and hence find the explicit bounds.

In addition, we have provided some specific examples where we find the combinations (that is, w_1 and w_2) of the original variables that satisfy a maximum principle. These examples include an analysis of the three-ion electroneutral PNP equations applicable for modeling ion transport in biological cells where it is essential for healthy cell function that ion concentrations remain within given ranges. A second example shows that in the case of the coupled Burgers' equations, the compatibility condition is not in general satisfied. However, there is a particular choice of parameter values for which two simple combinations of the original variables satisfy maximum (and minimum) principles.

In Sec. V, we have found a relationship between the two advection terms, $R(u, v)$ and $Q(u, v)$, that ensures that the techniques described in this paper can be used. Given an arbitrary $R(u, v)$, a compatible $Q(u, v)$ can be found using Eqs. (34) and (37). This still allows for a broad class of equations since, even once $R(u, v)$ has been fixed, there is still the freedom to choose two arbitrary functions of a single variable to construct $Q(u, v)$.

The theory developed here can be extended to higher dimensions by considering the advection terms as vector functions, $\mathbf{R}(u, v)$ and $\mathbf{Q}(u, v)$, so that

$$u_t = \nabla^2 u + \nabla \cdot \mathbf{R}, \quad v_t = \nabla^2 v + \nabla \cdot \mathbf{Q}.$$

In this case one can readily show that Eq. (9) still holds, while Eq. (10) is replaced by its vector equivalent given by

$$W_U W_V \mathbf{R}_U - W_U^2 \mathbf{R}_V + W_V^2 \mathbf{Q}_U - W_U W_V \mathbf{Q}_V = \mathbf{0}.$$

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