Boundary Conditions for Chromatography Reactors in a State Of Maximum Mixedness

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December 15, 1993

1 Introduction

Chemical reactors with identical residence time distributions (RTDs) can have different conversions due to different mixing patterns within the reactors. In 1959 Zwittering showed that the conversion in a reactor with a given RTD is bounded by the two extreme mixing cases of maximum mixedness (MM) and complete segregation [6]. Further, he presented a physical model based on plug flow reactors (i.e. reactors where the velocity of the flow down the reactor is independent of cross-sectional location) that would simulate the two mixing cases. In the case of maximum mixedness, the reactor is simulated by a plug flow reactor in which the reactants enter through each point down the length of the reactor at a rate determined by the RTD. (In complete segregation the reactants enter at the beginning of the plug flow reactor, and the products are removed from the reactor side). In 1983 Schweich applied Zwittering's model for maximum mixedness to an equilibrium chromatographic adsorption reactor [4]. This type of reactor contains an immobile adsorbing solid phase which is in chemical equilibrium with a mobile fluid phase. Schweich showed that the mass balance for this reactor leads to the following nonlinear conservation law:

$$-x^2\frac{\partial c(t,x)}{\partial x} = \frac{\partial f(c(t,x))}{\partial t} + h(x)[c(t,x) - g(t)] \qquad x \in (0,1], t \in (-\infty,\infty). \quad (1.1)$$

In the above equation, t is time, x is a nonuniform scaling of length down the reactor, c is solute concentration in the fluid phase, g is the concentration of the solution as it enters the reactor, f is defined by the equilibrium relationship between the two phases, and h is determined from the RTD. To solve this conservation law, the value of c at the beginning of the reactor (i.e. $x = 0$) must be known. Schweich suggests generalizing the method utilized by Zwittering to determine this boundary condition. Zwittering states that "for all normal cases" this boundary condition can be determined by setting the term with the x derivative to zero, and replacing $h(x)$ with $H \equiv \lim_{x\to 0} h(x)$:

$$0 = \frac{df(c(t,0))}{dt} + H[c(t,0) - g(t)] \qquad t \in (-\infty,\infty). \quad (1.2)$$

This paper will establish a method for proving the validity of Schweich's boundary condition when H is finite and non-zero. Further, it will show how this method can be extended to many cases where Schweich's method no longer works ($H = 0$ or ∞). To establish this method, we will begin in Section 2 by summarizing Schweich's derivation of the conservation law in (1.1) from the mass balance for the MM chromatographic reactor. In Section 3, the nature of the boundary condition problem will be discussed, and theorems about the boundary condition will be stated. Section 4 will introduce the method of generalized characteristics, which will form the basis for the proofs of the theorems presented in Section 5.

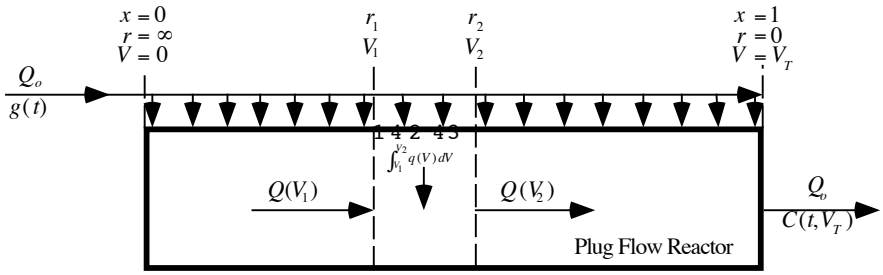

Figure 1: *Zwittering's model for reactors in a state of maximum mixedness. Solution of concentration $g(t)$ enters the reactor at constant total flow rate Q_o. The solution enters through each point on the side of the plug flow reactor at rate $q(V)$. V is the volume of the liquid in the reactor up to point V. r, the residence time, is the amount of time that solution entering at point r will remain in the reactor.*

2 Model Of The Physical System

We start with Zwittering's model for a MM reactor, which is shown in Figure 1. To compute $q(V)$, the rate at which the solution enters the reactor at point V, we need to use the residence time distribution, $E(r)$, which can be experimentally determined. The residence time distribution is defined as the fraction of the solution that stays in the reactor for exactly r units of time. (Therefore, $\int_0^\infty E(r)\,dr = 1$). $q(V)$ is related to $E(r)$ by the equation

$$q(V) = \frac{E(r)}{\int_r^\infty E(s)\,ds}. \tag{2.1}$$

$Q(V)$, the volumetric flow rate inside the reactor at point V, can be determined from $q(V)$ using

$$Q(V) = \int_0^V q(v)dv. \tag{2.2}$$

Finally, the relationship between r and V (both of which define location down the reactor) is given by

$$r = \int_V^{V_T} \frac{dv}{Q(v)}. \tag{2.3}$$

Now we are ready to look at the mass balance. Consider the case where the reactor shown in Figure 1 is filled with immobile, adsorbing solid particles in a manner that makes υ, the ratio of the solid phase volume over the liquid phase volume, constant throughout the reactor. Further, assume that the solid and liquid phases are always at chemical equilibrium, which allows us to state that n, the concentration of the solute in the solid phase, is strictly a function of C, the concentration of the solute in the liquid phase. A mass balance over a time interval, $[t_1, t_2]$, and volume interval, $[V_1, V_2]$, of the reactor — shown in Figure 1 — gives

us the equation

$$\int_{t_1}^{t_2}\int_{V_1}^{V_2} g(t)q(V)\,dV\,dt + \int_{t_1}^{t_2} C(t,V_1)Q(V_1)\,dt - \int_{t_1}^{t_2} C(t,V_2)Q(V_2)\,dt = \int_{V_1}^{V_2} C(t_2,V)+\upsilon n(t_2,V)\,dV - \int_{V_1}^{V_2} C(t_1,V)+\upsilon n(t_1,V)\,dV, \tag{2.4}$$

where the left side of the equation represents the number of moles of solute entering and leaving the volume segment, and the right side of the equation represents the accumulation of solute inside the volume segment. We apply the Gauss–Green theorem and the product rule to (2.4) to obtain

$$qg - \frac{dQ}{dV}C = Q\frac{\partial C}{\partial V} + \frac{\partial(C+\upsilon n)}{\partial t}. \tag{2.5}$$

Since n is strictly a function of C, we can define

$$f(C) = C + \upsilon n, \tag{2.6}$$

and using this definition along with the relations given in eqs. (2.1)–(2.3) we can transform (2.5) into

$$\frac{E(r)}{\int_r^\infty E(s)\,ds}[\overline{C} - g(t)] = \frac{\partial \overline{C}}{\partial r} - \frac{\partial f(\overline{C})}{\partial t} \text{ where } \overline{C}(t,r) = C(t,V). \tag{2.7}$$

For more details on this derivation see the papers by Zwittering and Schweich [4,6].

Because the range of the residence time, r, is inconvenient, we make one final substitution as suggested by Villermaux [5]:

$$x = \frac{1}{r+1}. \tag{2.8}$$

This leads to the final form of the mass balance:

$$-x^2\frac{\partial c}{\partial x} = \frac{\partial f(c)}{\partial t} + h(x)[c - g(t)] \qquad x \in (0,1], t \in (-\infty,\infty) \tag{2.9}$$

where $c(t,x) = \overline{C}(t,r)$ and $h(x) = \frac{E(r(x))}{\int_{r(x)}^\infty E(s)\,ds}$.

3 Determining The Proper Boundary Condition

The physical meaning of the functions $h(x)$, $g(t)$, $c(t,x)$, and $f(c)$ shown in the last section restricts these functions' possible behavior. Since $E(r)$, the residence time distribution, is nonnegative, $h(x)$ must also be nonnegative. Further, it is easily seen from its definition that $h(x)$ is a bounded function except possibly at $x = 0$. It is relatively easy to find RTDs that lead to $H \equiv \lim_{x\to 0} h(x)$ being infinite, positive, or zero as shown by Villermaux in [5]. $h(x)$ will also be assumed to be $C^1(0,1]$.

Since $g(t)$ is the concentration of the solution entering the reactor, $g(t)$ must be a nonnegative, bounded function. $g(t)$ is also assumed to be a C^1 function.

We will assume that $f(c) = c + \upsilon n(c)$ has the following two properties, which are usually physically justified: 1) There exist a, b such that $0 < a \leq b < \infty$ and $f'(c) \in [a, b]$ for $c \in [0, \|g\|]$ where $\|g\| = \sup_{t\in(-\infty,\infty)} g(t)$ and 2) $f(c)$ is C^2 and strictly concave. If the first property were false, there would have to be values of c where $n'(c)$ is negative. This would imply that a larger concentration in the liquid phase causes a smaller concentration in the solid phase, which is physically unlikely. Most equilibrium relations will also satisfy the second property since, according to DeVault's pioneering paper on the nature of chromatography [2], in "the usual type of equilibrium condition, $n''(c)$ is negative". The results of this paper will also be applicable in the case where f is strictly convex.

$c(t, x)$, the concentration of the liquid phase inside the reactor, cannot exceed the maximum concentration of the solution that has entered the reactor, so $g(t)$ bounds the behavior of $c(t, x)$ in the following sense:

$$0 \leq c(t, x) \leq \sup_{s\in(-\infty,t)} g(s) \leq \|g\|. \tag{3.1}$$

Because $f(c)$ is nonlinear, $c(t, x)$ may be discontinuous even when the boundary condition is smooth. It is necessary to make some assumptions about the nature of these discontinuities. First, we restrict $c(t, x)$ to be a function of locally bounded variation, which implies that for almost all fixed x, $c(t, x)$ is a function of locally bounded variation in t. In particular, for almost every fixed x and every t, $c(t, x)$ has limits from the left and the right: $c(t-, x)$ and $c(t+, x)$. In fact, it is known that $c(t-, x)$ and $c(t+, x)$ exist for every t and *every* x. We shall modify c to always equal its limit from the right; i.e. $c(t, x) = c(t+, x)$. From the theory of BV solutions it is known that this modification only involves altering c on a domain of measure zero. The solution to (2.9), even with a known boundary condition, is not unique. However, the physics of chromatography selects the unique solution that satisfies both (2.9) and, for concave f, the relation $c(t-, x) \leq c(t+, x)$ (see [3]). This relation is known as the entropy condition and is completely analogous to the entropy condition used in the study of shock waves in fluid dynamics.

If an arbitrary boundary condition $c^o(t) = c(t, 0)$ is specified, it is usually the case that no solution of the conservation law in (2.9) exists since the $x^2\frac{\partial c}{\partial x}$ term equals zero at $x = 0$. To remove this singularity, we modify the conservation law by slightly perturbing the x^2 factor:

$$-(x + \varepsilon)^2\frac{\partial c}{\partial x} = \frac{\partial f(c)}{\partial t} + h(x)[c - g(t)] \qquad x \in (0, 1],\ t \in (-\infty, \infty),\ \varepsilon > 0. \tag{3.2}$$

This perturbed form of the equation can be solved for any bounded, measurable boundary condition. Specifically, (3.2) can be solved for any arbitrary continuous boundary condition $c^o(t)$ where $c^o(t) \in [0, ||g||]$. We define the solution to the original conservation law (2.9) as the (pointwise) limit as ε approaches zero of

the solution to (3.2). The boundary condition for the original conservation law, $C^o(t)$, is defined as the limit of the solution of the original conservation law as x approaches zero:

$$C^o(t) = \lim_{x\to 0}\lim_{\varepsilon\to 0} c(t, x, \varepsilon, c^o(t)) \tag{3.3}$$

For $C^o(t)$ to be well defined, it will have to be independent of the choice of $c^o(t)$.

We can now formally state the results of this paper. For all four theorems $h(x)$, $g(t)$, $c(t, x)$, and $f(c)$ must have the properties stated in the preceding paragraphs of this section.

Theorem 3.1: *If $0 < H < \infty$, then the ordinary differential equation (1.2) has only one bounded C^1 solution, and the boundary condition $C^o(t)$ for (2.9) is equal to that solution.*

In other words, Schweich's generalization of Zwittering's method is confirmed for this case.

Theorem 3.2: *If $H = \infty$, then $C^o(t) = g(t)$.*

This allows the Schweich/Zwittering method to be extended to the cases where H is infinite.

Theorem 3.3: *If $H = 0$ and $\int_0^1 \frac{h(x)}{x^2}dx < \infty$, then $C^o(t)$ cannot be defined.*

As we will see later, in the case of Theorem 3.3, $C^o(t) = \lim_{t\to-\infty} c^o(t)$, but since this must hold for all admissible $c^o(t)$ (even those that don't have a limit), $C^o(t)$ does not make sense and cannot be defined.

Theorem 3.4: *If $H = 0$, $\int_0^1 \frac{h(x)}{x^2}dx = \infty$, and $\lim_{t\to-\infty} g(t)$ exists, then $C^o(t) = \lim_{t\to-\infty} g(t)$.*

The Schweich/Zwittering method allows for the boundary condition to be *any* constant. Theorem 3.4 makes the boundary condition unique by selecting the proper constant.

4 The Method Of Generalized Characteristics

To prove the theorems presented in Section 3, we will use results known from the theory of generalized characteristics. The reader can find the proofs to the theorems stated in this section and more details about the theory of generalized characteristics in the 1977 paper by Dafermos [1].

In a classical (C^1) solution to (3.2), a characteristic is defined as a path on the (t, x) plane that satisfies the ODE

$$\frac{dt}{dx} = \frac{f'(c(t, x))}{(x + \varepsilon)^2}. \tag{4.1}$$

The method of generalized characteristics allows us to extend the use of characteristics into regions of the (t, x) plane where the solution is no longer C^1. We begin with the definitions of a generalized characteristic and a backward characteristic:

Definition 4.1: *A Lipschitz continuous curve $t = \tau(x)$ defined on an interval of $[0, \infty)$ is a characteristic if for almost all x in the interval the following condition is satisfied:*

$$\tau'(x) \in \left[\frac{f'(c(\tau(x)+, x))}{(x+\varepsilon)^2}, \frac{f'(c(\tau(x)-, x))}{(x+\varepsilon)^2} \right]. \tag{4.2}$$

A backward characteristic through the point (t^o, x^o) is any characteristic through the point (t^o, x^o) that is defined on some interval $(s, x^o]$. The set of backward characteristics through a point form a funnel emanating from that point. This funnel is bounded by a minimal backward characteristic on the left of the funnel and a maximal backward characteristic on the right. These two characteristics behave as classical characteristics, as shown by the following definition and theorems. Both theorems depend crucially on the fact that $f(c)$ is concave.

Definition 4.2: *A characteristic, $\tau(x)$, defined on $[a, b]$ is called genuine if $c(\tau(x)-, x) = c(\tau(x)+, x)$ for almost all $x \in [a, b]$.*

Theorem 4.1: *For any $(t^o, x^o) \in (-\infty, \infty) \times (0, 1]$, the minimal and maximal backward characteristics through (t^o, x^o) are genuine.*

Theorem 4.2: *Let $t = \tau(x)$ be a genuine characteristic defined on $[a, b]$. Then there is a function $v(x)$ defined on $[a, b]$ so that $(\tau(x), v(x))$ is a continuously differentiable solution of the classical characteristic equations*

$$\tau'(x) = \frac{f'(v)}{(x+\varepsilon)^2} \tag{4.3a}$$

$$v'(x) = \frac{-h(x)[v - g(\tau(x))]}{(x+\varepsilon)^2} \tag{4.3b}$$

and $v(x) = c(\tau(x), x)$ for all $x \in (a, b)$. The minimal and maximal backward characteristics through (t^o, x^o) are determined by solving system (4.3) with initial conditions $(\tau(x^o), v(x^o)) = (t^o, c(t^o-, x^o))$ and $(\tau(x^o), v(x^o)) = (t^o, c(t^o+, x^o))$, respectively. The two characteristics coincide if and only if $c(t^o-, x^o) = c(t^o+, x^o)$.

The two theorems above can be used to provide the following corollary:

Corollary 4.1: *If the solution of the system of differential equations (4.3) through every point $(t^o, x^o, v^o) \in (-\infty, \infty) \times (0, 1] \times (-\infty, \infty)$ does not escape to $t = \pm\infty$ on $[0, x^o]$, then the backward characteristics through (t^o, x^o) are defined on $[0, x^o]$.*

Putting these theorems together with the restriction from Section 3 that $c(t, x) = c(t+, x)$ and the requirement that $c^o(t)$ be continuous, we know that the maximal

backward characteristic though (t^o, x^o), which we will denote as $\tau(x)$, and the concentration on that characteristic, $v(x)$, are determined by the solution of system (4.3) in the interval $x \in [0, x^o]$ with initial condition $(\tau(x^o), v(x^o)) = (t^o, c(t^o, x^o))$. This result will be used repeatedly in the proofs of the next section.

5 Proofs

We now use the results from the theory of generalized characteristics presented in Section 4 to prove the theorems stated in Section 3. Without loss of generality, we only consider the case where $t^o = 0$.

Theorem 3.1: *If $0 < H < \infty$, then the ordinary differential equation (1.2) has only one bounded C^1 solution, and the boundary condition $C^o(t)$ for (2.9) is equal to that solution.*

Proof: We begin by showing the existence and uniqueness of the bounded solution to (1.2),

$$0 = \frac{df(c)}{dt} + H[c - g(t)] \qquad t \in (-\infty, \infty). \tag{1.2}$$

Existence: We first rewrite (1.2) as

$$\frac{dc}{dt} = \frac{-H[c - g(t)]}{f'(c)} \qquad t \in (-\infty, \infty), \tag{5.1}$$

and consider this vector field on the (t, c) plane (Figure 2). In particular, we observe the behavior of the vector field on two domains

$$A = \{(t, c) \mid t \in (-\infty, 0], c \in [-\delta, \|g\| + \delta]\}$$

$$B = \{(t, c) \mid t \in [0, \infty), c \in [-\delta, \|g\| + \delta]\}$$

where δ is arbitrarily small. On the top and bottom edges of both domains the vector field points into the domain. On the line $t = 0$, the vector field points into domain B. From application of the Wazewski principle to domain A, we conclude that at least one trajectory must remain inside A for all negative times. Since this trajectory cannot escape through the top or the bottom of domain B, there must exist at least one trajectory of the vector field contained within $A \cup B$. Taking the limit as δ approaches zero, we conclude that there exists a solution of (1.2) such that $c \in [0, \|g\|]$ for all time.

Uniqueness: Since $f'(c) \in [a, b]$ where $a > 0$, we can define $f^{-1} = F$ where $F'(u) \in [1/b, 1/a]$. Setting $u = f(c)$, (1.2) is transformed into

$$\frac{du}{dt} = -H[F(u) - g(t)]. \tag{5.2}$$

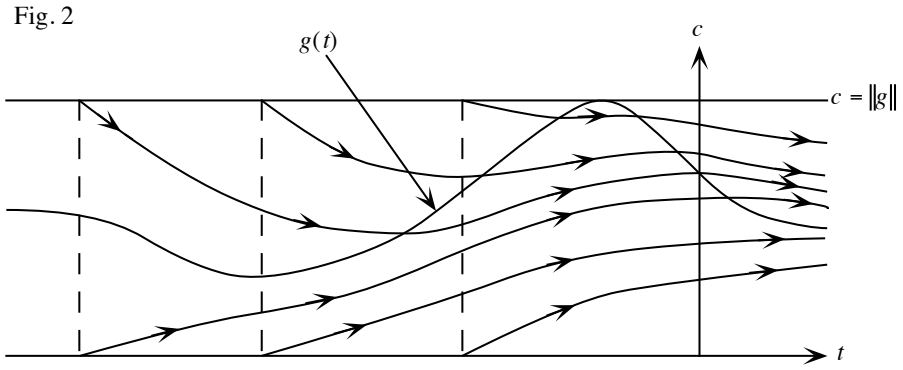

Figure 2: *Trajectories of the vector field* $\frac{dc}{dt} = \frac{-H(c-g(t))}{f'(c)}$. *Note how the trajectories pull closer as time progresses, forming nestled trajectory funnels.*

Assume there are two solutions, u_1 and u_2, such that both are bounded and $u_1 > u_2$. (Since (5.2) defines a flow, $u_1 > u_2$ for any value of t implies $u_1 > u_2$ for all values of t). It follows that

$$\frac{d(u_1 - u_2)}{dt} = -H[F(u_1) - F(u_2)] \leq -\frac{H}{b}(u_1 - u_2) \tag{5.3}$$

which, after integration between $t = -N$ and $t = 0$, yields

$$e^{\frac{HN}{b}}(u_1(0) - u_2(0)) \leq (u_1(-N) - u_2(-N)). \tag{5.4}$$

As N approaches infinity, one of the two solutions must diverge, but both solutions are supposed to be bounded. $\rightarrow\leftarrow$

Now it must be shown that the initial condition of Equation (2.9) is equal to the bounded solution of (1.2). First, we consider the behavior of $T(x; x^o, \varepsilon)$, the maximal backward characteristic emanating from the point $(0, x^o)$ for (3.2). Because $f'(c) \in [a, b]$, the behavior of $T(x; x^o, \varepsilon)$, which is described by (4.3a), is bounded by

$$-b\left[\frac{1}{(x+\varepsilon)} - \frac{1}{(x^o+\varepsilon)}\right] \leq T(x) \leq -a\left[\frac{1}{(x+\varepsilon)} - \frac{1}{(x^o+\varepsilon)}\right], \tag{5.5}$$

and, therefore, it follows that

$$\frac{-bx^o}{\varepsilon(x^o+\varepsilon)} \leq T(0) \leq \frac{-ax^o}{\varepsilon(x^o+\varepsilon)} \tag{5.6}$$

(see Figure 3). The evolution on the characteristic $T(x)$ of the concentration, which will be denoted as $V(T(x))$, is obtained by combining (4.3a) and (4.3b):

$$\frac{dV}{dT} = \frac{-h(x)[V - g(T)]}{f'(V)}. \tag{5.7}$$

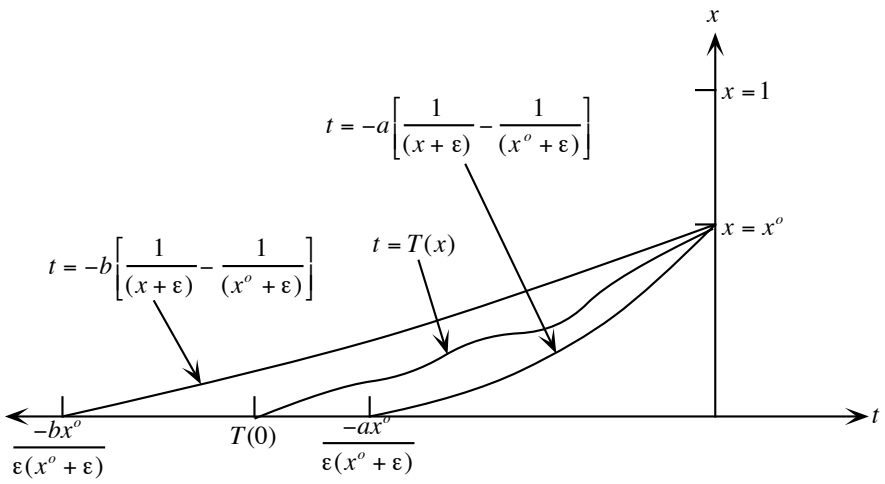

Figure 3: *The trajectory of the maximal backward characteristic, $T(x)$, and the bounds on its behavior. Note that as $\varepsilon \to 0$, $T(0)$ is forced to approach $-\infty$.*

Note that T is treated as an independent variable in (5.7), but it is also a function of x in the sense of (4.3a). Throughout this section the functionality of T will always be specified when $T(x; x^o, \varepsilon)$ is being discussed in the sense of (4.3a); otherwise T should be thought of as the independent variable in the sense of (5.7).

We wish to exploit the similarities between (5.7) and (5.1). Since $h(x)$ approaches H, we can define a small $E(x^o)$ such that $h(x) \in [H - E, H + E]$ for all $x \in [0, x^o]$. Now consider the behavior of the following three vector fields:

$$\frac{d\overline{V}}{dT} = \frac{-H[\overline{V} - g(T)]}{f'(\overline{V})} \tag{5.8a}$$

$$\frac{dv^l}{dT} = \begin{cases} \dfrac{-(H+E)[v^l - g(T)]}{f'(v^l)} & v^l \geq g(T) \\ \dfrac{-(H-E)[v^l - g(T)]}{f'(v^l)} & v^l < g(T) \end{cases} \tag{5.8b}$$

$$\frac{dv^u}{dT} = \begin{cases} \dfrac{-(H-E)[v^u - g(T)]}{f'(v^u)} & v^u \geq g(T) \\ \dfrac{-(H+E)[v^u - g(T)]}{f'(v^u)} & v^u < g(T) \end{cases} \tag{5.8c}$$

Given the same arbitrary initial condition, $(T(0), c^o(T(0)))$, for each field in (5.7) and (5.8), the relation $v^l(T) \leq V(T), \overline{V}(T) \leq v^u(T)$ holds. As ε approaches zero, $T(0; x^o, \varepsilon) \to -\infty$ (from (5.6)), so the domain of the vector fields approaches $T \in (-\infty, 0]$. The same existence and uniqueness arguments used previously

can be easily modified to show that as $\varepsilon \to 0$ the trajectory through the point $(T(0), c^o(T(0)))$ in each of the vector fields in (5.7) and (5.8) must converge, regardless of the choice of $c^o(t)$, to a unique bounded solution of each field on $T \in (-\infty, 0]$. Further, the unique solution of (5.8a) must be the same as the unique bounded solution to (1.2). All that remains is to show that $\lim_{x^o \to 0} \lim_{\varepsilon \to 0} (v^u(0) - v^l(0)) = 0$. This is accomplished with the method used previously in the uniqueness proof :

$$\frac{d(u^u - u^l)}{dT} = -H(F(u^u) - F(u^l)) + E(|v^u - g| + |v^l - g|)$$

$$\leq -\frac{H}{b}(u^u - u^l) + 4E\|g\|. \tag{5.9}$$

Combining the fact that $F'(u) \leq 1/a$ with the result obtained from multiplying (5.9) by the appropriate integrating factor and then integrating between $T = T(0)$ to $T = 0$ leads to

$$v^u(0) - v^l(0) \leq \frac{4b\|g\|E(x^o)}{aH} \quad \forall \varepsilon. \tag{5.10}$$

Applying both limits to (5.10) leads to the desired result since $\lim_{x^o \to 0} E(x^o) = 0$. This completes the proof of the theorem.

Theorem 3.2: *If $H = \infty$, then $C^o(t) = g(t)$.*

Proof: As in the proof of Theorem 3.1, when ε approaches zero, the trajectory of (5.7) through the point $(T(0), c^o(T(0)))$ defined on $T \in [T(0), 0]$ converges to the unique bounded solution of (5.7) defined on $T \in [-\infty, 0]$. As x^o approaches zero, the x^o dependent vector field defined by (5.7) on the (T, V) plane will have trajectories that diverge from $g(T)$ progressively faster (in negative time), which will force the unique bounded solution of (5.7) to be progressively closer to $g(T)$. This idea forms the basis for the remainder of the proof.

Since $g \in C^1$, we know that there exists a $K \geq 2$ such that $|g'(T)| \leq K$ for all $T \in [-\|g\|, 0]$. Further, for any large N, there exists a small enough x^o so that $h(x) \geq 2bN$ for all $x \in [0, x^o]$.

Let $V(0) - g(0) \geq 2K/N$. Using (5.7), this condition implies that

$$\left.\frac{d(V-g)}{dT}\right|_{T=0} \leq -K \quad \Rightarrow \quad \frac{d(V-g)}{dT} \leq -K \quad \forall T \in [-\|g\|, 0]. \tag{5.11}$$

Integration of (5.11) between $T = -\|g\|$ and 0 shows that $V(-\|g\|) \geq 2\|g\|$, which is impossible since concentration cannot exceed $\|g\|$. If $V(0) - g(0) \leq -2K/N$, a similar contradiction occurs. So we conclude that

$$|c(0, x^o) - g(0)| \leq \frac{2K}{N}. \tag{5.12}$$

As x^o approaches zero, N gets infinitely large, so c approaches g. This completes the proof of this theorem.

Theorem 3.3: *If $H = 0$ and $\int_0^1 \frac{h(x)}{x^2} dx < \infty$, then $C^o(t)$ cannot be defined.*

Proof: On the characteristic $T(x)$, we can define $G(x;x^o,\varepsilon) = g(T(x;x^o,\varepsilon))$ and $\hat{V}(x) = V(T(x))$, which allows (4.3b) to be expressed solely in terms of functions of x:

$$\hat{V}'(x) = \frac{-h(x)[\hat{V} - G(x)]}{(x+\varepsilon)^2}. \tag{5.13}$$

(5.13) can be solved for $\hat{V}$, which leads to the following expression for $\hat{V}(x^o) = c(0,x^o)$:

$$c(0,x^o) = A(x^o) + B(x^o)$$

$$\text{where } A(x^o) = c^o(T(0)) \exp\left[-\int_0^{x^o} \frac{h(s)}{(s+\varepsilon)^2} ds\right]$$

$$\text{and } B(x^o) = \int_0^{x^o} \frac{h(x)}{(x+\varepsilon)^2} G(x) \exp\left[\int_{x^o}^{x} \frac{h(s)}{(s+\varepsilon)^2} ds\right] dx. \tag{5.14}$$

We must determine the limit of (5.14) first as $\varepsilon \to 0$ and then as $x^o \to 0$. The term $B(x^o)$ is easily bounded:

$$B(x^o) \le \|g\| \left(1 - \exp\left[-\int_0^{x^o} \frac{h(s)}{(s+\varepsilon)^2} ds\right]\right). \tag{5.15}$$

Dominated convergence allows us to apply both limits to the integral in the exponential leading to the conclusion $\lim_{x^o\to 0} \lim_{\varepsilon\to 0} B(x^o) = 0$. Dominated convergence also implies that the exponential term in $A(x^o)$ converges to one when both limits are taken. Since $T(0) \to -\infty$ as $\varepsilon \to 0$, we find that

$$C^o(t) = \lim_{x^o\to 0} \lim_{\varepsilon\to 0} c(t,x^o) = \lim_{t\to-\infty} c^o(t). \tag{5.16}$$

But the value — and existence — of the limit on the right-hand side of (5.16) depends on the arbitrary choice of $c^o(t)$, which cannot be allowed in any reasonable definition of the boundary condition, $C^o(t)$. Therefore, no boundary condition may be defined in this case. This completes the proof of the theorem.

Theorem 3.4: *If* $H = 0$, $\int_0^1 \frac{h(x)}{x^2} dx = \infty$, *and* $\lim_{t\to-\infty} g(t)$ *exists, then* $C^o(t) = \lim_{t\to-\infty} g(t)$.

Proof: (5.14), used in the last theorem, is still valid, but it now shows the opposite behavior in the sense that $B(x^o)$ is the significant term and $A(x^o)$ converges to zero:

$$\lim_{\varepsilon\to 0} A(x^o) \le \|g\| \exp\left[-\int_0^{x^o} \frac{h(s)}{s^2} ds\right] = 0 \qquad \forall x^o. \tag{5.17}$$

$B(x^o)$ is determined by splitting the integration into two regions, $\left[0, \frac{ax^o}{a+Nx^o}\right]$ and $\left[\frac{ax^o}{a+Nx^o}, x^o\right]$ where N is a large fixed number. This will allow us to isolate the behavior on the part of the characteristic where T is very negative. For convenience we define

$$\Phi(x;x^o,\varepsilon) = \frac{h(x)}{(x+\varepsilon)^2} \exp\left[\int_{x^o}^{x} \frac{h(s)}{(s+\varepsilon)^2} ds\right], \tag{5.18}$$

which allows us to more compactly express the following bounds for $B(x^o)$:

$$\left[\inf_{x\in\left[0,\frac{ax^o}{a+Nx^o}\right]} G(x)\right]\int_0^{\frac{ax^o}{a+Nx^o}}\Phi(x)dx+\left[\inf_{x\in\left[\frac{ax^o}{a+Nx^o},x^o\right]} G(x)\right]\int_{\frac{ax^o}{a+Nx^o}}^{x^o}\Phi(x)dx\le B(x^o)\le$$

$$\left[\sup_{x\in\left[0,\frac{ax^o}{a+Nx^o}\right]} G(x)\right]\int_0^{\frac{ax^o}{a+Nx^o}}\Phi(x)dx+\left[\sup_{x\in\left[\frac{ax^o}{a+Nx^o},x^o\right]} G(x)\right]\int_{\frac{ax^o}{a+Nx^o}}^{x^o}\Phi(x)dx. \tag{5.19}$$

The monotone convergence and dominated convergence theorems are used to find the limits of the integral terms in (5.19):

$$\lim_{x^o\to 0}\lim_{\varepsilon\to 0}\int_{\frac{ax^o}{a+Nx^o}}^{x^o}\Phi(x)dx\le\lim_{x^o\to 0}\left[\max_{x\in[0,x^o]}h(x)\right]\frac{N}{a}=0 \tag{5.20}$$

$$\lim_{x^o\to 0}\lim_{\varepsilon\to 0}\int_0^{\frac{ax^o}{a+Nx^o}}\Phi(x)dx=\lim_{x^o\to 0}\exp\left[-\int_{\frac{ax^o}{a+Nx^o}}^{x^o}\frac{h(s)}{s^2}ds\right]=1. \tag{5.21}$$

The bounds on the behavior of the characteristic, $T(x)$, given in relation (5.5) combined with the continuity of g allow us to bound the other terms in (5.19):

$$\lim_{x^o\to 0}\lim_{\varepsilon\to 0}\left[\inf_{x\in\left[0,\frac{ax^o}{a+Nx^o}\right]} G(x)\right]\ge\lim_{x^o\to 0}\inf_{t\in(-\infty,-N)} g(t)=\inf_{t\in(-\infty,-N)} g(t) \tag{5.22}$$

$$\lim_{x^o\to 0}\lim_{\varepsilon\to 0}\left[\sup_{x\in\left[0,\frac{ax^o}{a+Nx^o}\right]} G(x)\right]\le\lim_{x^o\to 0}\sup_{t\in(-\infty,-N)} g(t)=\sup_{t\in(-\infty,-N)} g(t). \tag{5.23}$$

So (5.19) reduces to

$$\inf_{t\in(-\infty,-N)} g(t)\le\lim_{x^o\to 0}\lim_{\varepsilon\to 0} c(0,x^o)\le\sup_{t\in(-\infty,-N)} g(t). \tag{5.24}$$

Since N is arbitrarily large, we conclude

$$\lim_{x\to 0}\lim_{\varepsilon\to 0} c(0,x)=\lim_{t\to-\infty} g(t). \tag{5.25}$$

This completes the proof of the theorem.

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