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The propagation of reaction - diffusion waves in coupled autocatalytic systems

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Abstract

The initiation of reaction-diffusion travelling waves in two regions each governed by simple isothermal kinetics is considered when the two regions are coupled together. The basic reaction in each region is quadratic autocatalysis with the decay of the autocatalyst to an inert product in just one of the regions being allowed. The situation when the coupling is achieved via the reactant is discussed in detail and compared with previous results obtained when the coupling is via the autocatalyst. Substantial differences both in the conditions for the formation of travelling waves and in their ultimate propagation speed are seen between the two coupling mechanisms. The permanent-form travelling wave structure is shown to depend on the initial input of autocatalyst when the coupling is via the reactant, which is not the case when the coupling is via the autocatalyst.

1. Introduction

Recent experimental studies (Maselko and Showalter 1991, Winston et al. 1991, Gaspar et al. 1991) have begun to examine the coupling of chemical waves across membrane surfaces. Such systems are of interest, not least because of their implications for trans-membrance signalling in biological contexts.

These experiments typically make use of an ion-exchange membrane, such as Nafion, onto which one component of the reaction is selectively absorbed (and potentially immobilized). The remaining components are provided from the surrounding solution, which acts as a reservoir of these species, but these cannot all penetrate into the membrane due to electrostatic repulsion. Coupling from one side of the membrance to the other is achieved via the exchange of electrically neutral components, and the strength of the coupling can be controlled by varying the experimental conditions. The analogies between autocatalytic systems with chemical feedback and non-isothermal systems such as flames which rely on thermal feedback is also of relevance, as thermal coupling can readily be envisaged in the combustion context.

In a series of recent papers (Merkin et al. 1993, Metcalf et al. 1993, Needham and Merkin 1994) we have considered, in some detail, the initiation and propagation of reaction-diffusion waves in coupled isothermal autocatalytic systems. In particular, we considered the coupling of two reaction regions which we refer to as region I and region II. In region I we assumed an autocatalytic reaction, of the form

$$A + m\,B \rightarrow (m+1)\,B \qquad \text{rate} \quad k_1\,ab^m \tag{1a}$$

together with some autocatalyst decay or termination process, of the form

$$n\,B \rightarrow C \qquad \text{rate} \quad k_2\,b^n \tag{1b}$$

In region II we assumed that the reaction was purely autocatalytic, of the type given by step (1a). Throughout we assumed that the two regions were coupled together by the linear diffusive interchange of just one of the reactant species A or B.

In Merkin et al. (1993) we gave a systematic analysis of the case when there was quadratic autocatalysis (m=1) and linear decay (n=1) in region I and quadratic autocatalysis in region II, with the two regions being coupled via the autocatalyst B. We showed that conditions for the initiation of travelling waves depended on both the strength of the coupling between the two regions and on the strength of the decay step relative to the autocatalytic production step (characterized by dimensionless parameters γ_B and k respectively), but not on the initial input of B into the system provided it was not entirely non- trivial. We found that, when formed, the permanent-form travelling wave had an essentially new structure which could not be deduced directly from a knowledge of the wave forms that arise in each of the regions separately (when these are not coupled together). We also found that the propagation speed depended on both k and γ_B.

In the course of our discussion of the particular case mentioned above, we found that the linearized problem, based on small inputs of the autocatalyst B, could, when viewed in the appropriate way, provide clear insights into the conditions under which waves would be initiated as well as giving the propagation speeds of such waves. We extended this idea in Needham and Merkin (1994) to cases where there could be either quadratic or cubic autocatalysis (m=2) with either linear or quadratic decay (n=2) in region I coupled to either quadratic or cubic autocatalysis in region II. We found that the linearized theory could, in most cases, resolve the question as to the conditions under which waves could be formed and provided the appropriate propagation speed. These were found to depend on both the coupling strength parameter γ_B and the decay rate parameter k and were different in each of the cases considered. The case for which the basic linearized theory was inconclusive (cubic autocatalysis in regions I and II, with quadratic decay in region I) because of a zero eigenvalue was resolved by a consideration of the higher order terms in the expansion for small inputs.

In both the above papers the coupling between the two regions was through the autocatalyst B. The alternative configuration, where the coupling is achieved via reactant A, has been discussed in Metcalf et al. (1993) Here we considered two specific cases, namely the same case as in Merkin et al (1993) (quadratic autocatalysis in regions I and II with a linear decay step in I) and cubic autocatalysis with linear decay in region I with region II being unreactive, with reactant A being free to diffuse. When we come to compare the problems described in Merkin et al. and Metcalf et al. with the same kinetic mechanism we find that the mode of coupling has a major influence on both the conditions for the initiation of a travelling wave and on the structure and speed of the waves that form. As we have already mentioned, when the coupling is via autocatalyst B both the conditions for initiation of waves and their resultant speed and structure are strongly influenced by both the parameters γ_B and k. However, when the coupling is via reactant A we found that travelling waves are formed for all values of the relative decay strength parameter k and the coupling strength parameter γ_A. A further difference between the two systems is that the propagation speed is now independent of both k and γ_A, being the same as for the standard Fisher-Kolmogorov wave (see, for example, Britton, 1986) that would arise naturally in region II if this were decoupled from region I. The parameters k and γ_A do have an influence on the structure of the permanent-form travelling waves, with the concentration of autocatalyst B being identically zero in region I if $k \geq 1$, for all γ_A.

Further differences between the two methods of coupling regions I and II arise from how the travelling waves are initiated by the localized initial input of autocatalyst B. When the coupling is via autocatalyst B we found that the conditions for travelling waves to develop and the speed and structure of any such waves was independant of whether B was introduced into region I or region II (or both). However, when the coupling is via reactant A, the propagation speed and the structure of the waves that form depends crucially on whether the autocatalyst is introduced into region I or into region II.

The purpose of this paper is to emphasis the major differences that arise in reaction-diffusion waves governed by simple isothermal autocatalytic kinetics when the mode of coupling is through the autocatalyst, more of which is produced by the reaction, or by the reactant species, which is consumed by the reaction. We start by giving the equations for both cases. We then summarize the results given in Merkin et al. (1993) (for coupling through B) and then go on to describe the two, essentially different, permanent-form travelling wave structures that can arise when the coupling is through reactant A, depending on whether the autocatalyst is introduced initially into region II or not. One of these wave forms has been discussed by Metcalf et al. (1993) whereas the other is new.

2. Equations

Throughout we assume that there is quadratic autocatalysis with linear decay (steps 1a and 1b with m = n = 1) in region I and quadratic autocatalysis in region II.

(a) Coupling through autocatalyst B

The dimensionless equations for this case are, from Merkin et al (1993),

$$\frac{\partial \alpha_1}{\partial t} = \frac{\partial^2 \alpha_1}{\partial x^2} - \alpha_1 \beta_1 \tag{2a}$$

$$\frac{\partial \beta_1}{\partial t} = \frac{\partial^2 \beta_1}{\partial x^2} + \alpha_1 \beta_1 - k\beta_1 + \gamma_B (\beta_2 - \beta_1) \tag{2b}$$

$$\frac{\partial \alpha_2}{\partial t} = \frac{\partial^2 \alpha_2}{\partial x^2} - \alpha_2 \beta_2 \tag{2c}$$

$$\frac{\partial \beta_2}{\partial t} = \frac{\partial^2 \beta_2}{\partial x^2} + \alpha_2 \beta_2 + \gamma_B (\beta_1 - \beta_2) \tag{2d}$$

where the α_i and β_i (i = 1, 2) are the (dimensionless) concentrations of chemical species A and B respectively and the suffices refer to regions I and II.

(b) coupling through reactant A

Here the equations are, from Metcalf et al (1993),

$$\frac{\partial \alpha_1}{\partial t} = \frac{\partial^2 \alpha_1}{\partial x^2} - \alpha_1 \beta_1 + \gamma_A (\alpha_2 - \alpha_1) \tag{3a}$$

$$\frac{\partial \beta_1}{\partial t} = \frac{\partial^2 \beta_1}{\partial x^2} + \alpha_1 \beta_1 - k \beta_1 \tag{3b}$$

$$\frac{\partial \alpha_2}{\partial t} = \frac{\partial^2 \alpha_2}{\partial x^2} - \alpha_2\beta_2 + \gamma_A (\alpha_1 - \alpha_2) \tag{3c}$$

$$\frac{\partial \beta_2}{\partial t} = \frac{\partial^2 \beta_2}{\partial x^2} + \alpha_2\beta_2 \tag{3d}$$

In both cases the initial and boundary conditions are the same, namely

$$\alpha_i = 1, \; \beta_i = \begin{cases} \beta_0^{(i)} g_i(x) & |x| \le \sigma \quad \text{at } t = 0 \\ 0 & |x| > \sigma \end{cases} \tag{4}$$

$$\alpha_1 \to 1, \; \beta_i \to 0 \text{ as } |x| \to \infty \quad t \ge 0 \tag{5}$$

for i = 1, 2, where the $\beta_0^{(i)}$ are constants and the functions $g_i(x)$ are continuous and non-negative on $|x| \le \sigma$ with a maximum value of unity.

3. Coupling through the autocatalyst

The condition for the initiation of permanent-form travelling waves in the system described by equations (2) and initial-boundary conditions (4, 5) is that

$$k < \frac{2\gamma_B - 1}{\gamma_B - 1} \quad \text{for} \quad \gamma_B > 1 \tag{6}$$

whereas waves are initiated for all k if $\gamma_B \le 1$.

If we introduce the travelling co-ordinate

$$y = x - vt \tag{7}$$

where v is a (strictly) positive constant into equations (2), we obtain the equations for the permanent-form travelling waves as

$$\alpha_1'' + v\,\alpha_1' - \alpha_1\beta_1 = 0 \tag{8a}$$

$$\beta_1'' + v\beta_1' + \alpha_1\beta_1 - k\beta_1 + \gamma_B (\beta_2 - \beta_1) = 0 \tag{8b}$$

$$\alpha_2'' + v\alpha_2' - \alpha_2\beta_2 = 0 \tag{8c}$$

$$\beta_2'' + v\beta_2' + \alpha_2\beta_2 + \gamma_B (\beta_1 - \beta_2) = 0 \tag{8d}$$

(where primes denote differentiation with respect to y). The boundary conditions are:

$$\alpha_i \to 1, \quad \beta_i \to 0 \quad \text{as } y \to \infty \tag{9a}$$

and that conditions are uniform at the rear of the wave, which, in turn, implies that

$$\alpha_i \to \alpha_i^s \,, \quad \beta_i \to 0 \quad \text{as} \quad y \to -\infty \tag{9b}$$

(i = 1, 2), where the α_i^s are non-negative constants.

In Merkin et al. (1993) it was shown that a non-trivial solution of equations (8) required that the propagation speed v satisfies the inequality

$$v \geq v_{min} = \sqrt{2}\left(2\,(1-\gamma_B) - k + \sqrt{k^2 + 4\gamma_B^{\;2}}\right)^{1/2} \tag{10a}$$

with the permanent-form travelling wave which arises as the large time solution from initial conditions (4) , in fact, propagating with speed v_{min}. A further consideration of equations (8) showed that

$$\alpha_i > 0,\ \beta_i > 0 \text{ on } -\infty < y < \infty \ (i = 1,\ 2) \tag{10b}$$

Consequently, the structure of permanent-form travelling waves which can arise will be such that the concentrations of both reactant A and autocatalyst B will be strictly non-zero in each region. This result is independent of how the waves are started i.e., whether one of $\beta_0^{(1)}$ or $\beta_0^{(2)}$ is zero. It is this result we compare with the case when the coupling is through reactant A, which we discuss in the next section. Finally, we note that inequality (10b) can be improved to

$$\alpha_i^s < \alpha_i < 1 \quad \text{on } -\infty < y < \infty,\ (i = 1,\ 2) \tag{10c}$$

4. Coupling through reactant A

Here we start by considering the reaction - diffusion system given by equations (3) and initial-boundary conditions (4, 5).

(a) initial-boundary value problem

We have already established in Metcalf et al. (1993) the bounds

$$0 \leq \alpha_i\ (x,t) \leq 1, \quad 0 \leq \beta_i\ (x,t) \leq 2 + \beta_0^{(1)} + \beta_0^{(2)}\ (i = 1,2) \tag{11a}$$

for $-\infty < x < \infty$, $t \geq o$. A consequence of (11a) is that the initial-boundary value problem (3,4,5) has a unique global solution. We have also established that when $k \geq 1$,

$$\beta_1\ (x,t) \to 0 \text{ uniformly in } x \text{ as } t \to \infty \tag{11b}$$

We now consider the nature of the solution of the initial-value problem if either $\beta_0^{(1)} = 0$ or $\beta_0^{(2)} = 0$. We start by considering the case $\beta_0^{(2)} = 0$, i.e. we assume there is no initial input of autocatalyst into region II. If we consider the scalar parabolic operator defined by

$$L\left[W\right] \equiv W_t - W_{xx} - W \qquad (12a)$$

then it is straightforward to show that

$$L\left[0\right] = 0, \qquad L\left[\beta_2\right] = -(1 - \alpha_2)\,\beta_2 \le 0 \qquad (12b)$$

from (11a). Also, with $\beta_0^{(2)} = 0$,

$$\beta_2\,(x,0) = 0 \text{ for all } x \qquad (12c)$$

and hence by the comparison theorem (for, example, Britton, 1986) we have

$$\beta_2\,(x,\ t) \le 0, \quad -\infty < x < \infty, \quad t \ge 0 \qquad (12d)$$

This leads, from (11a), to

$$\beta_2\,(x,\ t) \equiv 0 \quad \text{if} \quad \beta_0^{(2)} = 0 \qquad (13a)$$

By a similar argument, it follows that

$$\beta_1\,(x,\ t) \equiv 0 \quad \text{if} \quad \beta_0^{(1)} = 0 \qquad (13b)$$

Results (13) show that if no autocatalyst is introduced into either region initially then the concentration of the autocatalyst remains zero in that region throughout.

Now suppose $\beta_0^{(2)} > 0$ and consider the function $u_2(x,\ t)$ which satisfies the diffusion equation and the same initial - boundary conditions as β_2, namely

$$D\left[u_2\right] = 0 \qquad (14a)$$

$$u_2\,(x,\ 0) = \begin{cases} \beta_0^{(2)} g_2\,(x) & |x| \le \sigma \\ 0 & |x| > \sigma \end{cases} \qquad (14b)$$

$$u_2 \to 0 \text{ as } |x| \to \infty \qquad (14c)$$

where D [.] is the scalar diffusion operator

$$D[W] = W_t - W_{xx} \qquad (14d)$$

It is straightforward to write down the solution of (14) using Fourier transforms. The main point to note from this solution is that, since $\beta_0^{(2)}>0$, $u_2\,(x,\ t) > 0$ for $-\infty < x\ \infty$, $t \ge 0$. Then

$$D\left[u_2\right] = 0, \quad D\left[\beta_2\right] = \alpha_2\beta_2 \geq 0 \tag{15a}$$

$$u_2\ (x,\ 0) = \beta_2\ (x,\ 0) \tag{15b}$$

and hence, by the comparison theorem,

$$\beta_2\ (x,\ t) \geq u_2\ (x,\ t) > 0 \text{ for } -\infty < x < \infty,\ t \geq o \tag{16}$$

We now discuss the consequences of results (13) and (16) on the permanent-form travelling waves that can arise as long time solutions to initial - boundary value problem (3, 4, 5).

(b) Permanent-form travelling waves

On introducing the travelling co-ordinate y, given by (7), the equations for the permanent-form travelling waves are:

$$\alpha_1'' + v\ \alpha_1' - \alpha_1\beta_1 + \gamma_A\ (\alpha_2 - \alpha_1) = 0 \tag{17a}$$

$$\beta_1'' + v\ \beta_1' + \alpha_1\beta_1 - k\beta_1 = 0 \tag{17b}$$

$$\alpha_2'' + v\ \alpha_2' - \alpha_2\beta_2 + \gamma_A\ (\alpha_1 - \alpha_2) = 0 \tag{17c}$$

$$\beta_2'' + v\beta_2' + \alpha_2\beta_2 = 0 \tag{17d}$$

The boundary conditions ahead of the wave are

$$\alpha_i \to 1,\ \beta_i \to 0 \text{ as } y \to \infty\ (i = 1,\ 2) \tag{18}$$

When we consider the conditions that must apply at the rear of the wave (where conditions must become uniform) we find that there are two possibilities, namely either

$$\alpha_i \to 0\ (i, = 1,2),\ \beta_1 \to 0,\ \beta_2 \to B_s, \text{ as } y \to -\infty \tag{19a}$$

or

$$\alpha_i \to A_s,\ \beta_i \to 0\ (i = 1,2) \text{ as } y \to -\infty \tag{19b}$$

where $A_s \geq 0$ and $B_s \geq 0$ are constants. Thus we are looking for a non-negative, nontrivial solution to equations (17) subject to boundary conditions (18) and (19a) or (19b).

We first observe from equation (17d) that, whenever boundary conditions (19b) apply, $\beta_2(y) \equiv 0$ on $-\infty < y < \infty$, since, in this case,

$$\int_{-\infty}^{\infty} \alpha_2\ (y)\ \beta_2\ (y)\ dy = 0$$

It then follows, since $\alpha_2(y) > 0$ from Metcalf et al (1993), that $\beta_2(y) \equiv 0$.

We now discuss the structure that permanent-form travelling waves take for different initial input conditions. Consider first the case $\beta_0^{(2)} > 0$ and $\beta_0^{(1)} > 0$, i.e. some autocatalyst is introduced into both regions. Now, from (3d), we have, in the initial-value problem,

$$\frac{d}{dt}\int_{-\infty}^{\infty} \beta_2(x,t)\, dx = \int_{-\infty}^{\infty} \alpha_2(x,t)\beta_2(x,t)\, dx \geq 0 \tag{19c}$$

via (11a). Therefore

$$\int_{-\infty}^{\infty} \beta_2(x,t)\, dx \geq \beta_0^{(2)} \int_{-\sigma}^{\sigma} g_2(x)\, dx \equiv M > 0 \tag{19d}$$

for all $t > 0$. We conclude that $\beta_2(x,t)$ does not tend to zero uniformly in x as $t \to \infty$ as this would violate (19d). Hence, in this case, any travelling wave which forms from the initial-value problem must be a travelling wave satisfying conditions (19a) as $y \to -\infty$ (with $B_s > 0$). This is the situation that was analysed in Metcalf et al (1993). Here we showed that B_s, the concentration of B at the rear of the wave in region II satisfies

$$B_s > 0 \text{ with } B_s = 2 \text{ if } k \geq 1 \tag{20a}$$
$$B_s < 2 \text{ if } k < 1$$

We also showed that $\beta_1 \equiv 0$ if $k \geq 1$ and that the wave speed v satisfies the inequality

$$v \geq v_{min} = 2 \tag{20b}$$

Further consideration of the full initial-boundary value problem (3, 4, 5) then revealed that the permanent-form waves do, in fact, ultimately travel with their minimum possible speed i.e., their wave speed approaches $v_{min} = 2$ as $t \to \infty$.

Next consider the case when $\beta_0^{(2)} = 0$ (with $\beta_0^{(1)} > 0$ to achieve a wave at all). Here we have, from (13a), that $\beta_2 \equiv 0$ in the wave and it is boundary conditions (19b) that must apply. We are able to establish general properties of the travelling waves that arise in this case:

R1. No travelling wave exists with $\alpha_i \equiv 1$ ($i = 1, 2$).

Follows directly from Metcalf et al. (1993)

R2. In the travelling wave $\alpha_i(y) > 0$ on $-\infty < y < \infty$ $(i = 1, 2)$.

Follows directly from Metcalf et al. (1993)

R3. No travelling wave exists with $\beta_1 \equiv 0$.

With both $\beta_1 \equiv 0$ and $\beta_2 \equiv 0$ equations (17) reduce to a pair of coupled second order linear equations, from which it is readily shown that the only solution which satisfies boundary conditions (18, 19b) is the trivial solution $\alpha_1 \equiv 1$, $\alpha_2 \equiv 1$.

From this result we can conclude that any permanent-form travelling wave must have some range of y over which $\beta_1(y) > 0$ and we can then extend this result to.

R4. In the travelling wave $\beta_1(y) > 0$ for $-\infty < y \leq \infty$.

Suppose β_1 becomes zero at a finite value of $y = y_0$ (say), then, since we require a non-negative solution, we must have $\beta_1'(y_0) = 0$. Now, for a given $\alpha_1(y)$, equation (17) is a second order linear homogeneous equation with no singularities on $-\infty < y < \infty$. Thus any initial-value problem has a unique global solution on $-\infty < y < \infty$ (see for example, Grimshaw, 1990) ,. The above conditions on β_1 at y_o provide initial conditions for the unique global solution $\beta_1 \equiv 0$, and by R3 only the trivial solution is then possible.

Hence we must have $\beta_1(y) > 0$ on $-\infty < y < \infty$.

R5. In the travelling wave $\alpha_i(y) < 1$, $(i = 1, 2)$ on $-\infty < y < \infty$.

Putting $\phi = \alpha_1 + \alpha_2$, equations (17a, c) give

$$\phi'' + v\,\phi' = \alpha_1\,\beta_1 \tag{21a}$$

which can be integrated to give

$$\phi' = e^{-vy}\int_y^\infty \alpha_1\beta_1\,ds \tag{21b}$$

Then, from R2 and R4, $\phi' > 0$ and hence

$$2A_S < \alpha_1 + \alpha_2 < 2 \tag{21c}$$

Now suppose that $\alpha_1(y) \geq 1$ for some range of y. From boundary conditions (18, 19b) and ineqality (21c) α_1 must have a local maximum on this range, at $y = y_1$ (say), with then $\alpha_1(y_1) \geq 1$, $\alpha_1'(y_1) = 0$, $\alpha_1''(y_1) \leq 0$, $\alpha_2(y_1) < 1$. However, equation (17a) gives

$$\alpha_1''(y_1) = \alpha_1(y_1)\,\beta_1(y_1) + \gamma_A(\alpha_1(y_1) - \alpha_2(y_1)) > 0 \qquad (21d)$$

This is a contradiction and hence we must have $\alpha_1(y) < 1$ on $-\infty < y < \infty$. A similar argument applied to equation (17d) gives $\alpha_2(y) < 1$ on $-\infty < y < \infty$. This result can be extended to

R6. In the travelling wave $A_s < \alpha_2(y)$ on $-\infty < y < \infty$.

Suppose there is a finite range of y over which $\alpha_2(y) \leq A_s$, then there must be at least one value of y, y_2 (say), at which α_2 takes a local minimum, i.e, $\alpha_2(y_2) \leq A_S$, $\alpha_2'(y_2) = 0$, $\alpha_2''(y_2) \geq 0$ and, from (21c) $\alpha_1(y_2) > A_s$. Equation (17d) gives

$$\alpha_2''(y_2) = \gamma_A(\alpha_2(y_2) - \alpha_1(y_2)) < 0 \qquad (22)$$

This is a contradiction and the result then follows

R7. $A_s < 1$

This is clear from inequality (21c)

R8. A travelling wave exists only if $k < 1$.

Apply $\int^{\infty} \ldots dy$ to equation (17b) and boundary conditions (19b) to get

$$\int_{-\infty}^{\infty} (\alpha_1 - k)\,\beta_1\,dy = 0 \qquad (23a)$$

Using R5, we get

$$0 = \int_{-\infty}^{\infty} (\alpha_1 - k)\beta_1 dy \;<\; (1 - k)\int_{-\infty}^{\infty} \beta_1 dy \qquad (23b)$$

From which it follows, using R4, that we must have $k < 1$.

R9. The wave speed v satisfies $v \geq v_{min} = 2\sqrt{1-k}$.

For y large, equation (17b) can be linearized to:

$$\beta_1'' + v\,\beta_1' + (1-k)\,\beta_1 = 0 \tag{24a}$$

The solution to equation (24a) involves functions of the form $e^{\lambda_i y}$ where

$$\lambda_i = \frac{1}{2}\left(-v \pm \sqrt{v^2 - 4\,(1-k)}\right) \tag{24b}$$

For non-negative solutions we must have $v \geq 2\sqrt{1-k}$ and the result follows.

We can use the argument given in Merkin et al. (1989) to show that, for initial data with compact support, the permanent-form travelling wave which evolves as the large time solution of the initial-boundary value problem will travel with its minimum possible speed, i.e., the wave speed $v = v_{min} = 2\sqrt{1-k}$. We note that the propagation speed in this case is different to the case treated by Metcalf et al. (1993), where $\beta_0^{(2)} > 0$. There it was found that the waves had a propagation speed given by (20b).

Finally, we consider the case when $\beta_0^{(1)} = 0$ (and $\beta_0^{(2)} > 0$). Here $\beta_1 \equiv 0$ and $\beta_2 > 0$ in the wave and the results follow directly from Metcalf et al. (1993) . The behaviour in this case is analogous to the case when $k \geq 1$, discussed in this paper.

Further insights into the structure of the permanent-form travelling waves can be gained by looking for a solution of equations (17), with $\beta_2 \equiv 0$, for γ_A large and γ_A small. We start with the case γ_A large. Here an examination of equations (17) shows that $\alpha_2 \to \alpha_1$ in the limit as $\gamma_A \to \infty$. This suggests looking for a solution, valid for γ_A large, in the form

$$\alpha_i = A_0 + \gamma_A^{-1}\,\alpha_{i,1} + \ldots \quad (i = 1,\ 2) \tag{25a}$$
$$\beta_1 = \beta_{1,0} + \gamma_A^{-1}\,\beta_{1,1} + \ldots$$

At leading order, we obtain from equation (17b)

$$\beta_{1,0}'' + v\,\beta_{1,0}' + A_0\beta_{1,0} - k\beta_{1,0} = 0 \tag{25b}$$

At $O(\gamma_A^{-1})$ we obtain, from equations (17a,c)

$$\alpha_{1,1} - \alpha_{2,1} = A_0'' + v\,A_0' - A_0\beta_{1,0} \tag{26a}$$

$$\alpha_{2,1} - \alpha_{1,1} = A_0'' + v\, A_0' \tag{26b}$$

From which it follows that

$$A_0'' + v\, A_0' - \frac{1}{2} A_0 \beta_{1,0} = 0 \tag{26c}$$

On putting $\beta_{1,0} = 2\, \bar{\beta}_{1,0}$ (26c) gives the same equations (subject to the same boundary conditions) that were treated in detail by Merkin et al. (1989).

For strong coupling the concentrations of reactant A in both regions become equal with the wave propagating as though region I were decoupled from region II, though with double the concentration of autocatalyst in this region.

For weak coupling, $\gamma_A \ll 1$, and equations (17) suggest looking for a solution in this case by expanding

$$\alpha_i = \alpha_{i,0} + \gamma_A\, \alpha_{i,1} + \ldots \qquad (i = 1,\ 2) \tag{27}$$

$$\beta_1 = \beta_{1,0} + \gamma_A\, \beta_{1,1} + \ldots$$

At leading order we obtain

$$\alpha_{2,0} = 1 \tag{28a}$$

with $\alpha_{1,0}$, $\beta_{1,0}$ satisfying the equations

$$\alpha_{1,0}'' + v\, \alpha_{1,0}' - \alpha_{1,0}\beta_{1,0} = 0 \tag{28b}$$

$$\beta_{1,0}'' + v\, \beta_{1,0}' + \alpha_{1,0}\beta_{1,0} - k\, \beta_{1,0} = 0 \tag{28c}$$

together with the boundary conditions

$$\alpha_{1,0} \to 1,\ \beta_{1,0} \to 0 \text{ as } y \to \infty,\ \alpha_{1,0} \to \alpha^s,\ \beta_{1,0} \to 0 \text{ as } y \to -\infty \tag{28d}$$

The solution of these equations has been discussed in detail by Merkin et al. (1989), where it was shown that a solution exists for all $k < 1$ and $v \geq 2\sqrt{1-k}$, with $\alpha_{1,0}$ satisfying the inequality $0 < \alpha^s < \alpha_{1,0} < 1$.

Expression (28a) shows that a non-uniformity develops in the solution as $y \to -\infty$ (as the boundary conditions (19b) are not fully satisfied). To obtain further information about this non-uniformity we need to consider the equations of $O(\gamma_A)$ in expansion (27). These equations are linear and the details of their solution is not important, except for the behaviour as $y \to -\infty$. We find that

$$\alpha_{1,1} \sim -\frac{(1-\alpha_s)}{v} y, \quad \beta_{1,1} \to 0, \quad \alpha_{2,1} \sim \frac{(1-\alpha_s)}{v} y \tag{29}$$

as $y \to -\infty$, where α_s is known from the solution at leading order. Expression (29) suggest that we need an outer region of thickness $0(\gamma_A^{-1})$ at the rear of this region, in which we put

$$Y = \gamma_A y, \quad \alpha_1 = A_1(Y), \quad \alpha_2 = A_2(Y), \quad \beta_1 \equiv 0 \tag{30}$$

At leading order the equations satisfied by A_1 and A_2 are

$$vA'_1 + A_2 - A_1 = 0 \tag{31a}$$

$$vA'_2 + A - A_2 = 0$$

subject to, from (28d, 29)

$$A_1 \sim \alpha_s - \frac{(1-\alpha_s)}{v} Y + \ldots, \quad A_2 \sim 1 + \frac{(1-\alpha_s)}{v} Y + \ldots \tag{31b}$$

as $Y \to 0$. The solution of equations (31a) which satisfies the matching conditions (31b) is readily found to be

$$A_1 = \frac{(1+\alpha_s)}{2} - \frac{(1-\alpha_s)}{2} \exp(2y/v), \quad A_2 = \frac{1+\alpha_s}{2} + \left(\frac{1-\alpha_s}{2}\right) \exp(2y/v) \tag{32}$$

From (32) we have $A_S = \frac{1}{2}(1+\alpha_s)$ at the rear of the wave, with this limiting form being approach from above by α_2 but from below by α_1. This shows that, at least for γ_A small, there will be a region of the wave where $\alpha_1 < A_s$.

(c) Numerical results

(i) Initiation in one or both regions

The initial-boundary value problem (3,4,5) and the permanent-form travelling wave equations (17) were integrated numerically to illustrate the various differences in behaviour detailed above. We integrated equations (3, 4, 5) with $\gamma_A = 0.5$, $k = 0.5$, $\beta_0^{(1)} = 1.0$ and with $\beta_0^{(2)} = 0.01$ and with $\beta_0^{(2)} = 0.0$. The results are shown in figure 1, in which we plot the position of the travelling front (where α_1 (x,t) = 0.5) for the two cases. We can see that the propagation speed v(t) rapidly approaches a constant (straight line) in both cases. However, this speed is different in the two cases, v(t) → 2 when $\beta_0^{(2)}$ = 0.01 as t → ∞, whereas for $\beta_0^{(2)}$ 0.01, v(t) approaches a value which correlates well with $2\sqrt{1-k}$ for t large. Thus we see that the final speed of the wave depends on whether reaction is initiated only in region I or in both regions. In the latter case, we would obtain wave fronts in both regions in the absence of coupling, one propogating with speed v = $2\sqrt{1-k}$ (region I) and the other (region II) with speed v = 2. When these are coupled, the higher speed wave in region II determines the velocity in the overall system. For the case $\beta_0^{(2)}$ = 0, there would be no wave in region II in the absence of coupling and the natural speed for the wave in region I is v = $2\sqrt{1-k}$ as before. In the present case, the two regions are coupled through exchange of the reactant A, so even with the coupling no autocatalyst is produced in region II and hence there is no actual ‘reaction event’ in this region. Depletion of the reactant in this case arises only through the loss by exchange into the rear of the wave in region I.

(ii) Wave Profiles: strong coupling

We next considered the structure of the permanent-form travelling waves that emerge as long time solutions of the initial-value problem. In figure 2 we show results for k = 0.5 and γ_A= 5.0. We took $\beta_0^{(2)}$ = 1.0 for figure 2a and $\beta_0^{(2)}$ = 0.0 for figure 2b (in both cases $\beta_0^{(1)}$ = 1.0). For this value of γ_A the α_1 and α_2 profiles are virtually indistinguishable in either figure (as suggested by the large γ_A analysis) but these profiles are different in the two cases. In figure 2a the α_i → 0 at the rear of the wave (boundary condition (19a)) whereas in figure 2b they approach a non-zero constant (boundary condition (19b)). In the first case β_2 undergoes a large excursion in the wave with β_1 being very small throughout (being too small to register on the scale for figure 2a). In the second case, where β_2 ≡ 0, β_1 achieves much higher values in the wave. Thus we again see that there are important differences between the wave structures emerging in the two cases $\beta_0^{(2)} > 0$ and $\beta_0^{(2)} = 0$.

(iii) Wave profiles: intermediate coupling

In figures 3 we plot the permanent-form wave structure when $\gamma_A = 1.0$, $k = 0.5$, $\beta_0^{(1)} = 1.0$, $\beta_0^{(2)} = 0.0$ to compare with figure 2b. The only change between these two figures is the reduction in γ_A and this shows itself through a slight separation in the α_1 and α_2 wave profiles.

(iv) Wave profiles: weak coupling

We next took a much smaller value of γ_A. In figure 4 we plot wave profiles for $\gamma_A = 0.1$ and $k = 0.5$, the only differences between the two figures being that for figure 4a we took $\beta_0^{(2)} = 1.0$ and for figure 4b we took $\beta_0^{(2)} = 0.0$ so different wave structures emerge in the two cases. The α_1 and α_2 profiles are now much more distinct and at the rear of the wave approach zero in figure 4a but approach a non-zero constant (somewhat larger than previously seen) in figure 4b. Again, the β_1 profile is very small throughout in the first case, but attains appreciable values in the second ($\beta_2 \equiv 0$ in the second case, whereas it undergoes a large variation in the first.) One feature to note about the α_1 profile shown in figure 4b is, as predicted by the small γ_A analysis, the final value at the rear of the wave is approached from below. This is even more clearly seen in figure 5, where we take $\gamma_A=0.01(k=0.5, \beta_0^{(1)}=1.0, \beta_0^{(2)}=0.0)$.

Finally we examined the structure of the permanent-form waves when the value of k is reduced. These are shown in figure 6 where we take $k = 0.1$ and $\beta_0^{(1)} = 1.0$. In both cases $\beta_0^{(2)} = 0$ and $\beta_2 \equiv 0$ throughout. Comparing figure 6a ($\gamma_A = 5.0$) with figure 2b we can see that the main difference in reducing k is to greatly increase the values reached by β_1 and to decrease the values reached by the α_i at the rear of the wave. Now we also see that β_1 can achieve values greater than unity, which it cannot do in the uncoupled system as was shown in Merkin et al (1989) that $\beta_1 < 1$ in the wave. The same general trends are seen when we compare figures 6b ($\gamma_A = 0.1$) and figure 4b, though now β_1 remains less then unity in the wave.

5. Conclusion

We have considered the possible initiation of travelling waves in a coupled reaction - diffusion system goverened by simple isothermal kinetics. We took two parallel plane regions with autocatalytic (or chain - branching) reactions taking place in both, the difference between the two regions being that in one region we allowed the autocatalyst to decay to some inert product whereas this reaction step was not present in the other. The main purpose of our analysis is to compare the conditions under which travelling waves form and the wave structure of any such waves, when the coupling between the two regions is achieved either through the reactant (which is used up in the autocatalytic reaction) or through the autocatalyst (which is produced by the autocatalytic reaction and is used up in the decay step).

When the coupling takes place via the autocatalyst we found conditions which involved both the relative decay rate strength k and coupling rates γ_B for waves to form. These are given by expression (6). We also found that the propagation speed of any waves that form involves both γ_B and k, as given by expression (10a). A further feature of this case is that the initiation and propagation speed of the travelling waves is independent of how the autocatalyst is introduced into the system (into an otherwise uniform expanse of reactant).

Considerable and important differences are seen when we consider the regions being coupled via the reactant. The conditions for the initiation of waves and their ultimate propagation speed depend on how the autocatalyst is introduced initially into the system. If some autocatalyst is introduced into both regions, then travelling waves form for all values of the decay rate parameter k and coupling strength γ_A. In this case the waves propagate with an asymptotic wave speed $v_0 = 2$ (in dimensionless units). However, if the autocatalyst is not introduced into the region without the decay step, travelling waves form only if $k < 1$ (for all values of γ_A), with the further difference being that the asymptotic wave speed $v_0 = 2\sqrt{1-k}$ in this case.

Further differences are seen when we come to compare the structure of the permanent-form travelling waves that are initiated. When the coupling is via the autocatalyst, the concentration profiles of the autocatalyst are pulse-like, approaching zero at the rear of the wave, while the concentrations of the reactant approach differnt (constant) non-zero values at the rear of the waves. When the coupling is via the reactant, the structure of the permanent-form travelling waves depends on how they were initiated. When some autocatalyst is introduced into both regions, the concentration profiles of the reactant and of the autocatalyst in one region all approach zero at the rear of the wave, while the concentration profile of the autocatalyst in the other region approaches a (relatively large) constant value. When the autocatalyst is introduced into just the one region, the concentration of the autocatalyst in the other region remains zero throughout and essentially different permanent-form wave structures are seen. The non-zero autocatalyst concentration is pulse-like, but now the concentrations of the reactant approach the same (constant) non-zero value at the rear of the wave.

The fact that we find essentially different behaviour between the two coupling mechanisms is, perhaps, not entirely unexpected. We have already observed differences in coupled well-stirred (spatially uniform) systems governed by cubic autocatalator kinetics, Leach et al. (1991, 1992) when the coupling is via the reactant or via the autocatalyst. However, the fact that we get essentially different asymptotic structures (permanent-form travelling waves) depending on how these waves are initiated is novel and, perhaps, unexpected as this feature has not been observed in all our previous studies on reaction - diffusion travelling waves.

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Captions for figures

Figure 1 Position of the travelling front plotted against t obtained from a numerical integration of equations (3,4, 5) with $\gamma_A = 0.5$, $k = 0.5$, $\beta_0^{(1)} = 1.0$ for $\beta_0^{(2)} = 0$ and $\beta_0^{(2)} = 0.01$.

Figure 2 Permanent - form travelling waves for $\gamma_A = 5.0$, $k = 0.5$ and $\beta_0^{(1)} = 1.0$ with (a) $\beta_0^{(2)} = 1.0$, (b) $\beta_0^{(1)} = 0.0$.

Figure 3 Permanent - form travelling wave for $\gamma_A = 1.0$, $k = 0.5$, $\beta_0^{(1)} = 1.0$ and $\beta_0^{(2)} = 0.0$.

Figure 4 Permanent - form travelling waves for $\gamma_A = 0.1$ $k = 0.5$ and $\beta_0^{(1)} = 1.0$ with (a) $\beta_0^{(2)} = 1.0$, (b) $\beta_0^{(2)} = 0.0$.

Figure 5 Permanent - form travelling wave for $\gamma_A = 0.01$, $k = 0.5$, $\beta_0^{(1)} = 1.0$, $\beta_0^{(0)} = 0.0$

Figure 6 Permanent - form travelling waves for $k = 0.1$, $\beta_0^{(1)} = 1.0$, $\beta_0^{(2)} = 0.0$ and (a) $\gamma_A = 5.0$, (b) $\gamma_A = 0.1$

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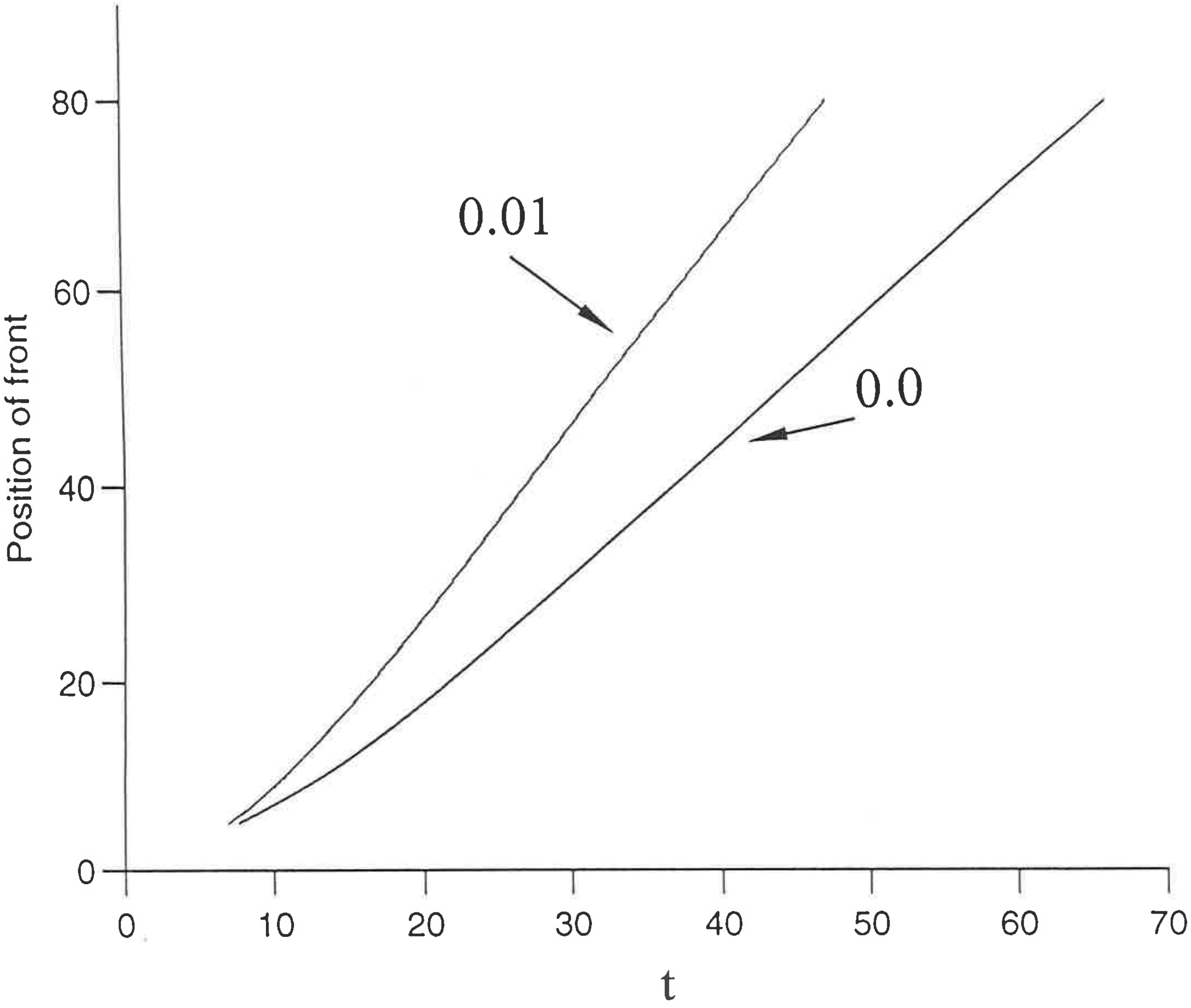

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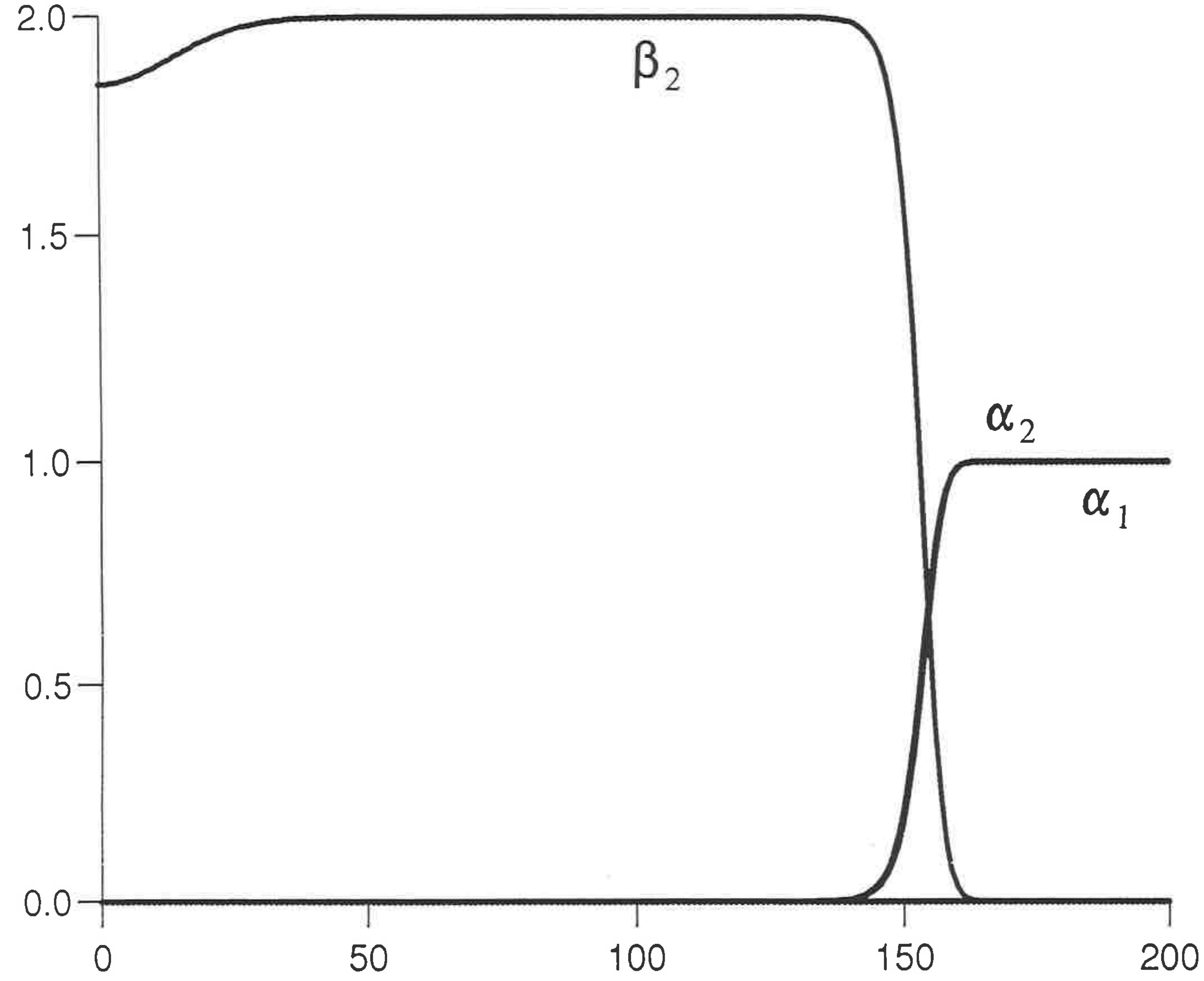

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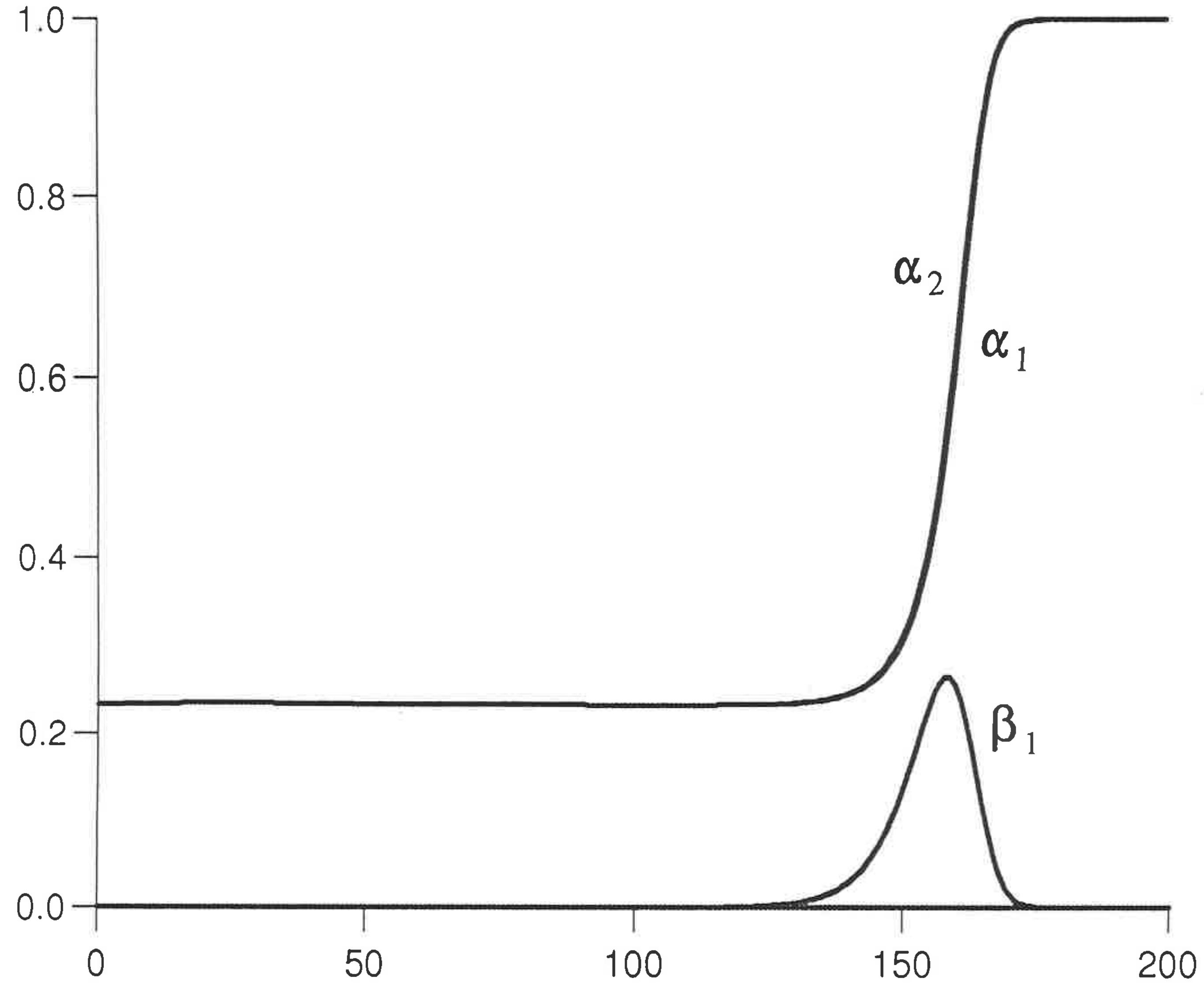

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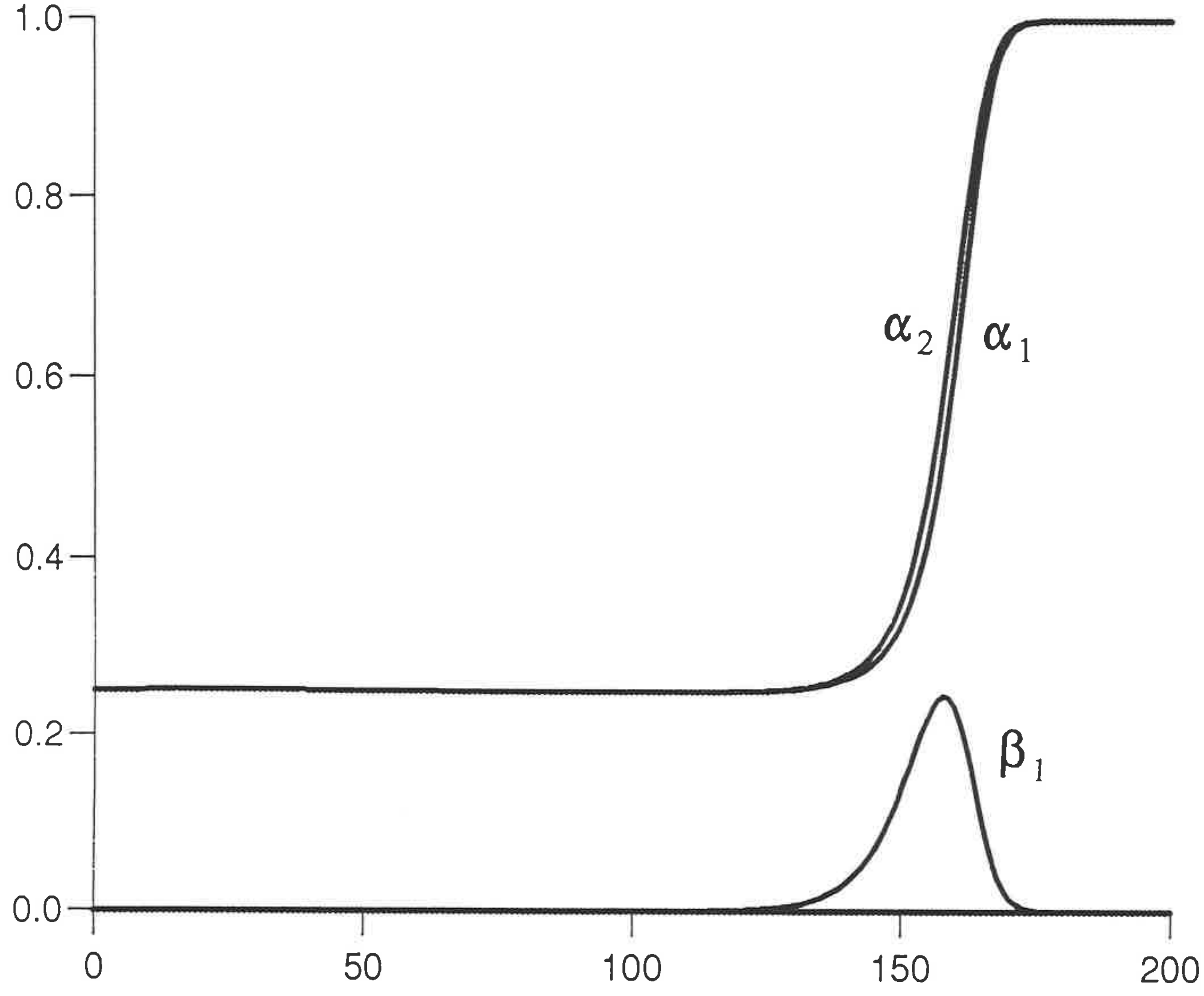

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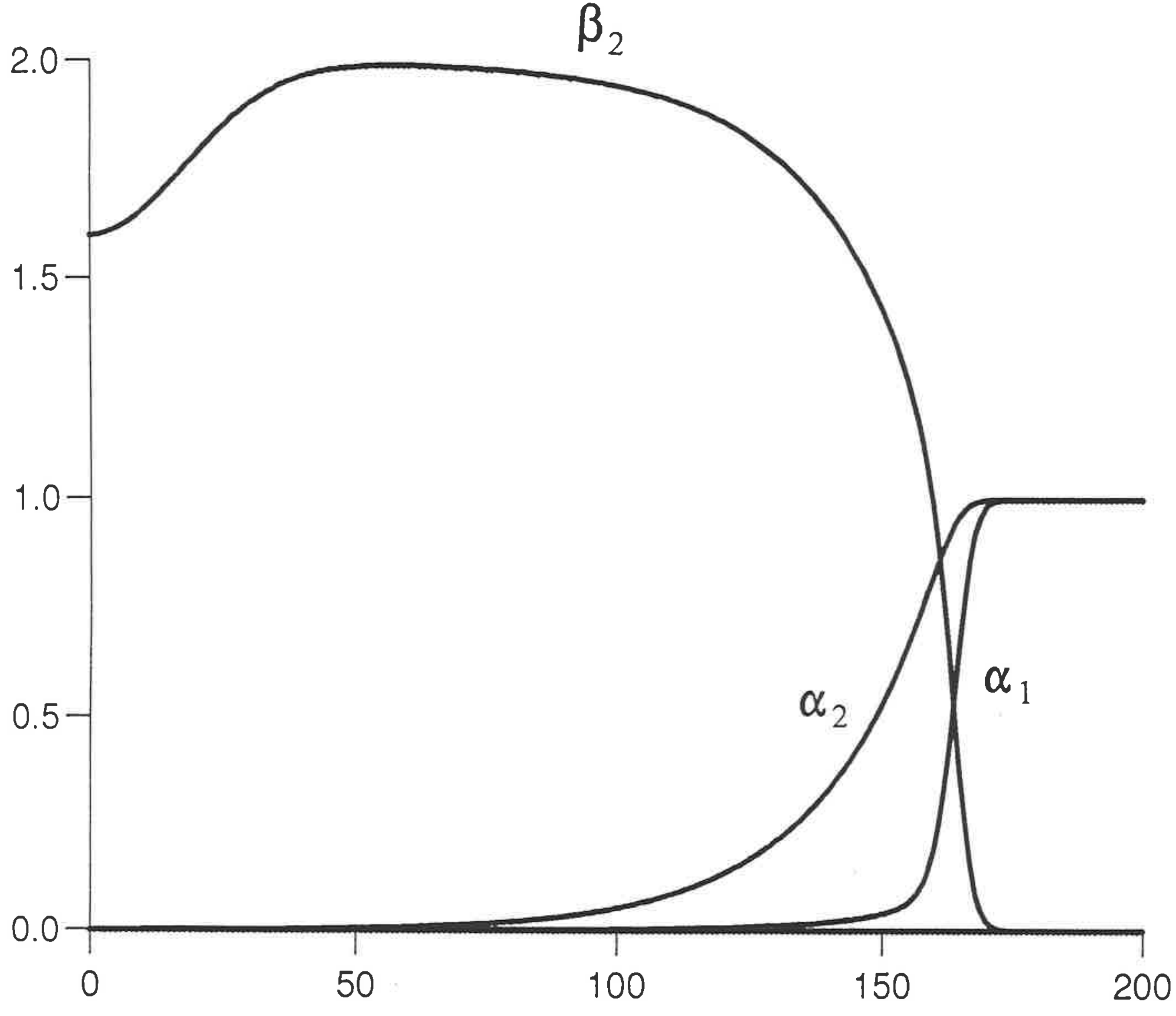

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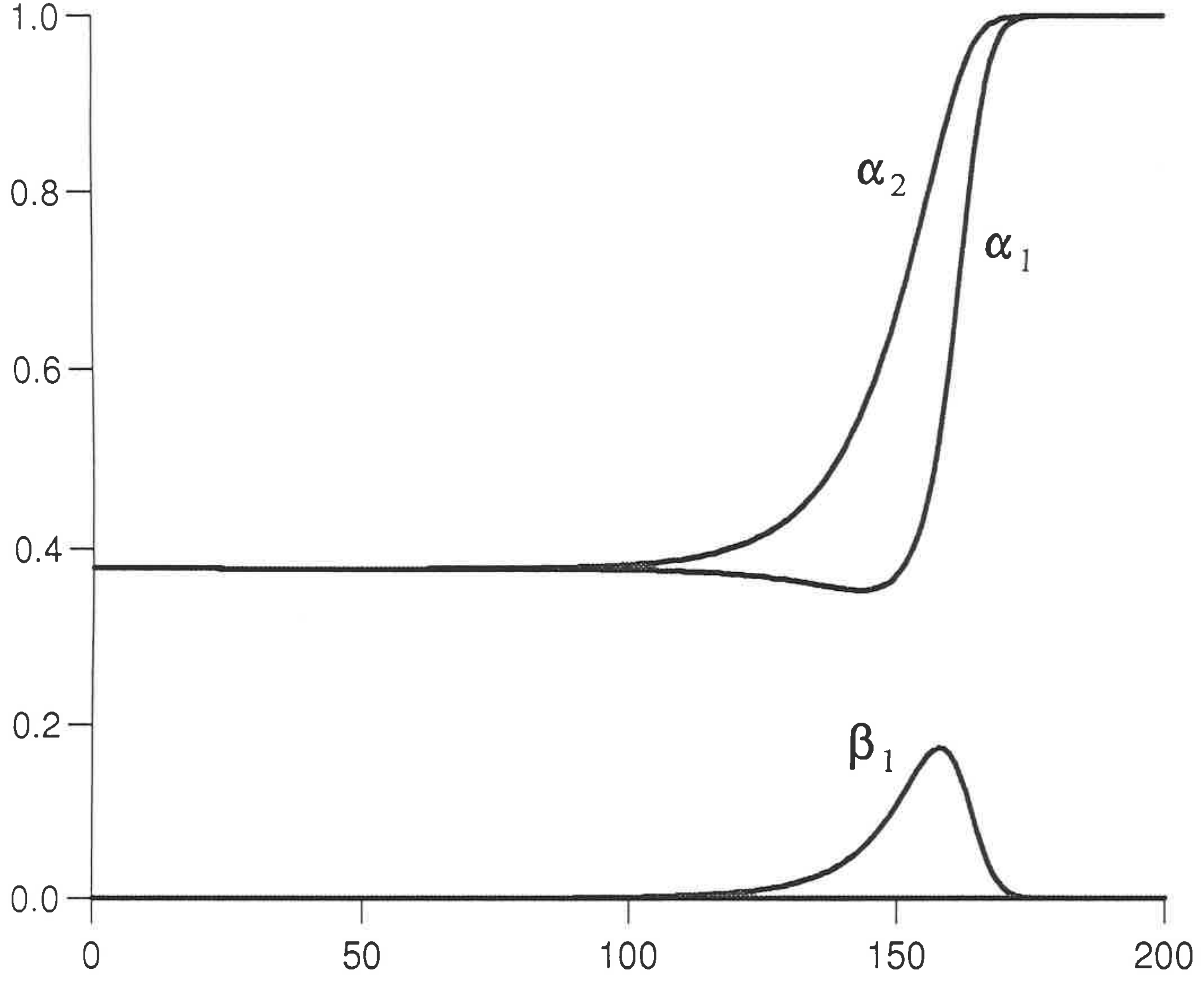

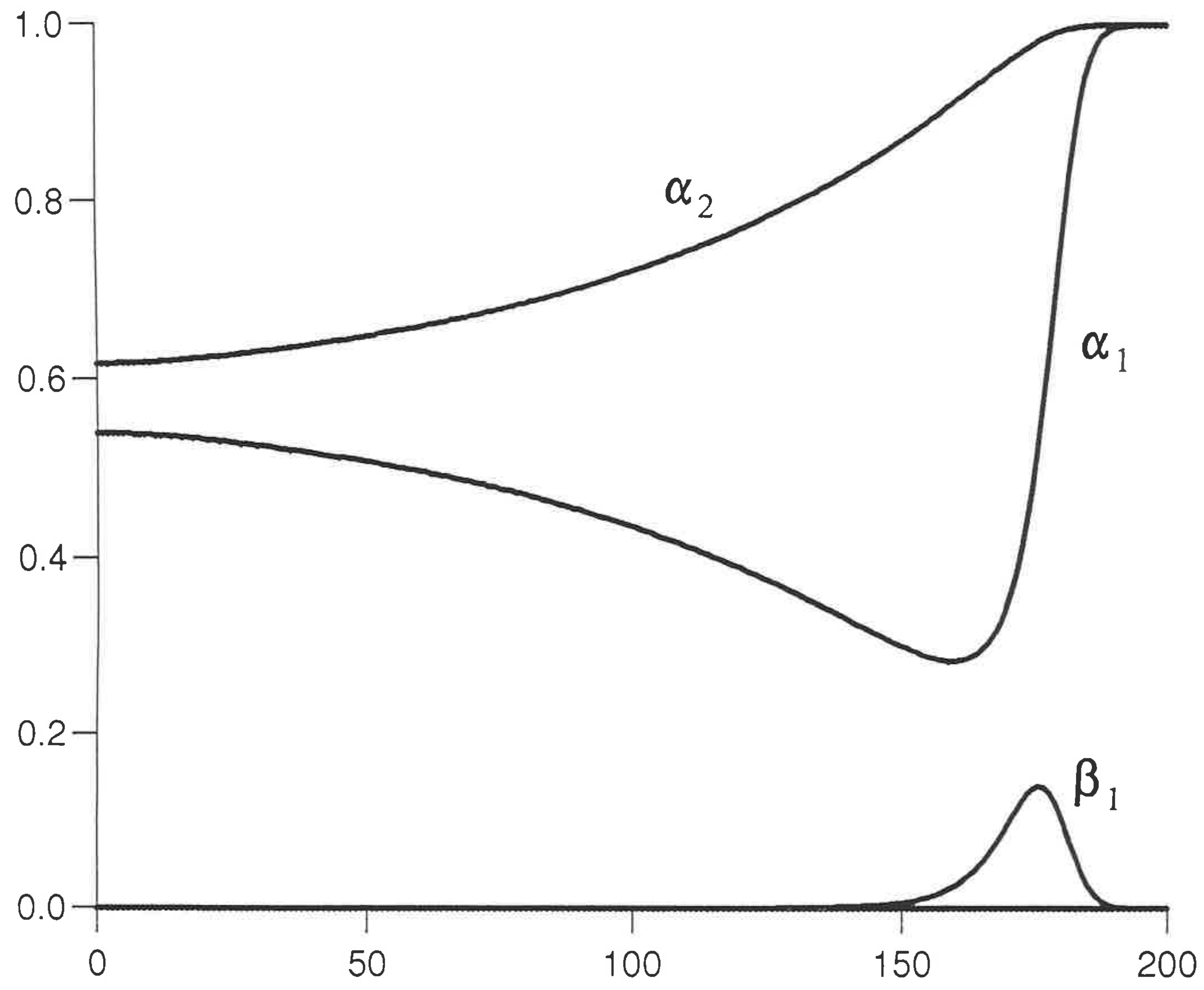
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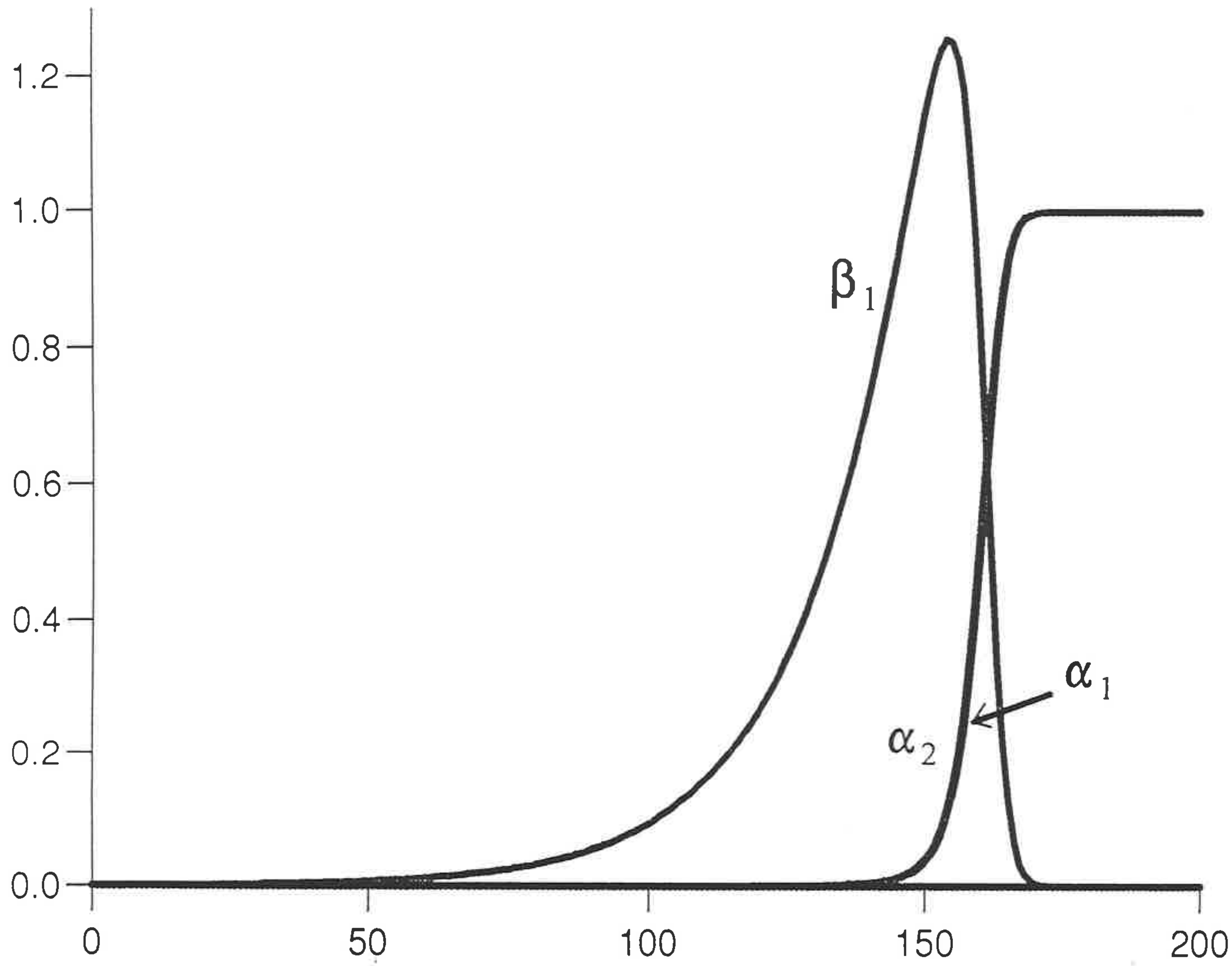
α_2
α_1
β_1

6a



6b