

CONF-880802--12

DE90 006313

## CHAPTER 7

## THE STOCHASTIC FLAMELET MODEL OF TURBULENT PREMIXED COMBUSTION\*

## ABSTRACT

A new stochastic model is presented and used to calculate the properties of turbulent premixed flames in the flame-sheet regime. The flame sheet is represented statistically by infinitesimal flamelets, each of which is characterized by its position, its unit normal vector, and its (infinitesimal) area. The evolution of the position and normal are completely determined by the fluid velocity and its spatial derivatives following the flamelet, which are modelled by stochastic processes. The flamelet area changes by stretching caused by velocity gradients, by the propagation of cusps, and because of curvature. An additional model is developed to account for the latter two mechanisms.

The Stochastic Flamelet Model is used in conjunction with the joint pdf approach to make calculations of non-stationary, statistically-plane turbulent premixed flames. These calculations demonstrate the practicality of the method and illustrate its attributes. Because it contains a natural and comprehensive statistical description of the flame sheet, the model allows the essential physical processes to be incorporated in a straightforward manner.

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\* This Chapter was taken from the paper by S.B. Pope, W.K. Cheng in the Twenty-Second Symposium (Int.) on Combustion, Seattle, 1988. Aug. 14-19

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FG02-86ER13553

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## INTRODUCTION

Both in spark ignition engines and in laboratory flames, turbulent premixed combustion most often occurs in the flame-sheet regime<sup>1-3</sup>. A thin flame sheet (thinner than the Kolmogorov scale) forms a surface<sup>4,5</sup> — possibly highly corrugated — that separates reactants from products (see Fig. 1). This flame surface is convected, bent and strained by the turbulence<sup>6</sup> and propagates (relative to the reactants ahead) at a speed that can depend on the local conditions.

A wide variety of modelling approaches has been applied to turbulent premixed flames in the flame-sheet regime. Some (e.g. refs. 7-9) aim at calculating global quantities — turbulent flame speed, overall mass-burning rate, etc. — while others (e.g., refs. 10-14) are more comprehensive in that they attempt to describe the temporal and spatial variations of statistics through the flame. Both the Bray-Moss-Libby model<sup>10,11</sup> and the pdf method<sup>12-14</sup> (which are in the latter category) have been successful in accounting for some of the experimental observations related to counter-gradient diffusion and flame-generated turbulence<sup>11,14</sup>. But both models have shortcomings in determining the local burning rate. In the Bray-Moss-Libby model the local burning rate is not determined at all<sup>11</sup>, and so the turbulent flame speed is required as an input to the calculation rather than emerging as a calculated result. In the pdf method the local burning rate is calculated, but not in an entirely satisfactory manner: the burning rate is (implicitly) assumed to be inversely proportional to the turbulent time scale<sup>12,15</sup>, and the incorporation of the influence of the laminar flame speed is ad hoc<sup>13</sup>.

The Stochastic Flamelet Model, presented here, provides a method for determining the local burning rate. It does so by explicitly representing the flame sheet and the processes that affect its evolution. The numerical implementation of the model is a Monte Carlo method in which the flame sheet is represented by large numbers of flame elements, or flamelets. Each flamelet has a position, an orientation and an (infinitesimal) area, which evolve according to stochastic models.

The Stochastic Flamelet Model is used in conjunction with the pdf method<sup>15</sup>, there being a two-way coupling between the two methods. A modelled equation is solved for the joint pdf of velocity, dissipation and reaction progress variable, the local mean reaction rate being supplied by the flamelet model. The pdf method determines the mean fields — velocity, progress variable etc. — required by the flamelet model.

The model is described in the next section. Calculations have been performed for the idealized case of an initially plane flame sheet in constant-density, stationary, isotropic turbulence. These calculations, reported in the third section, prove the practicality of the model and illustrate the influence of the laminar flame speed. Conclusions are drawn in the final section.

### THE STOCHASTIC FLAMELET MODEL

An infinitesimal flame element — or, flamelet — has position  $\underline{X}(t)$ , area  $dA(t)$ , and unit normal  $\underline{N}(t)$  (pointing into the reactants). By definition<sup>6</sup>, as it evolves, the flamelet remains part of the flame sheet by its position changing according to the equation

$$\dot{\underline{X}}(t) = \underline{U}(t) + w \underline{N}(t) . \quad (1)$$

Here  $\underline{U}(t)$  is the fluid velocity just ahead of the flame, and  $w$  is the local propagation speed of the flame-sheet relative to the reactants. In the present work we take  $w$  to be a constant — the laminar flame speed — but there is no difficulty in allowing for a dependence on the local strain rate.

In the variable-density case, the Eulerian velocity  $\underline{u}(\underline{x},t)$  is discontinuous at the flame sheet<sup>5</sup>. Hence, since  $\underline{U}(t)$  and  $w$  are defined with respect to the reactants, we have

$$\underline{U}(t) = \lim_{y \rightarrow 0} \underline{u}(\underline{X}(t) + |y| \underline{N}(t), t) . \quad (2)$$

In the constant-density case considered here  $\underline{u}(\underline{x},t)$  is continuous, and Eq. (2) reduces to  $\underline{U}(t) = \underline{u}(\underline{X}(t), t)$ .

The initial condition for Eq. (1) is of great importance. Let  $S_0$  denote the flame surface at the initial time  $t_0$ . Then the initial flamelet position  $\underline{X}_0 = \underline{X}(t_0)$  is a random variable uniformly distributed on  $S_0$ . Let  $A_0$  be the expected†initial surface area, and let  $dA_0$  be the initial (infinitesimal) area of the flamelet (i.e.  $dA(t_0) = dA_0$ ). We define

$$A(t) \equiv dA(t)/dA_0, \quad (3)$$

to be the area amplification of the flamelet.

From these definitions and a knowledge of the flamelet properties much useful information can be obtained<sup>6</sup>. The total expected surface area is

$$A_s(t) = A_0 \langle A(t) \rangle, \quad (4)$$

and, most importantly, the expected surface-to-volume ratio is

$$\Sigma(\underline{x}, t) = A_0 \langle A(t) \delta(\underline{x} - \underline{X}(t)) \rangle. \quad (5)$$

The importance of the surface-to-volume ratio stems from the following expression for the local expected burning rate  $\omega(\underline{x}, t)$  (volume burned per unit volume per unit time):

$$\omega(\underline{x}, t) = w \Sigma(\underline{x}, t). \quad (6)$$

Referring to Fig. 1, this formula can be understood by considering the volume  $V$  centered on the point  $\underline{x}$ . On a given realization let  $A_v(t)$  be the area of the surface within  $V$  at time  $t$ . ( $A_v(t)$  may well be zero.) In the infinitesimal time interval  $dt$ , the volume of fluid burned by the propagating surface within  $V$  is  $wA_v dt$ . Hence the volume-average burning rate is  $wA_v/V$ . Equation (6) is then obtained as

$$\begin{aligned} \omega(\underline{x}, t) &= \lim_{V \rightarrow 0} \langle wA_v/V \rangle \\ &= w \Sigma(\underline{x}, t). \end{aligned}$$

In addition to the equation for  $\underline{X}(t)$  (Eq. 1), evolution equations for  $\underline{N}(t)$  and  $A(t)$  can be derived from first principles<sup>6</sup>. They are:

$$\dot{N}_i = N_i N_j N_k U_{j,k} - N_j U_{j,i}, \quad (7)$$

†If the initial flame sheet varies from one realization to the next,  $S_0$  is a random surface, and  $A_0$  is a random variable.

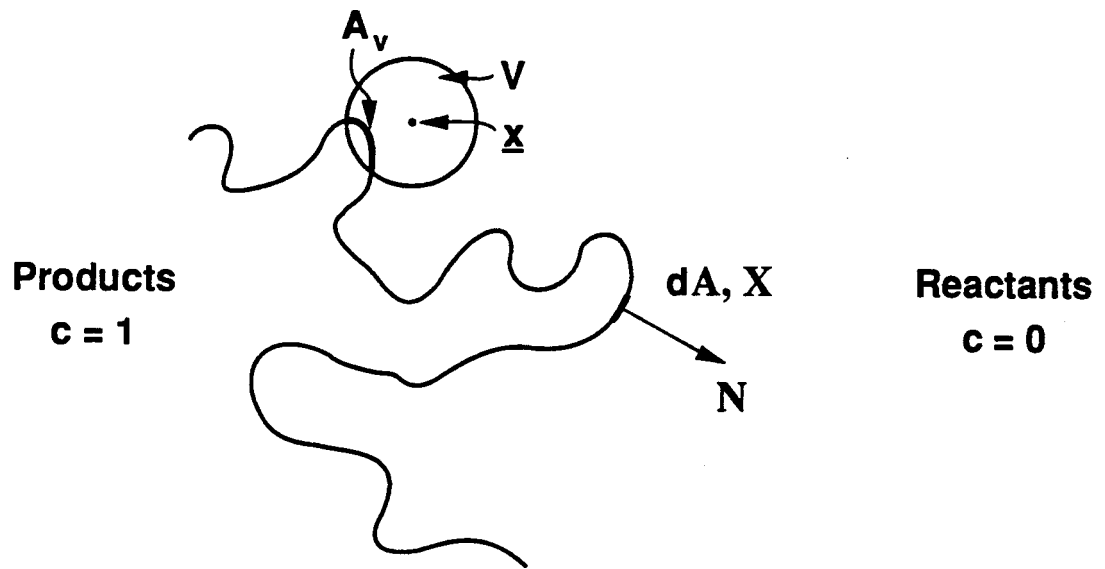


Figure 1: Sketch of a Flame Sheet.

$$\text{and } \dot{A} = -A N_i N_j U_{ij} - \dot{A}_R, \quad (8)$$

where  $U_{ij}$  denotes the velocity derivative  $\partial u_i / \partial x_j$  in the reactants just ahead of the flamelet. The initial condition  $\underline{N}(t_0)$  is determined by the initial orientation of the flamelet, while we have (from Eq. 3)  $A(t_0) = 1$ . The term  $\dot{A}_R$  is discussed at length below. For the moment we just observe<sup>6</sup> that it is zero for the case of a material surface ( $w=0$ ).

It is worth mentioning that the equations obtained depend on few assumptions: Eqs. (1-3) are definitions; while Eqs. (4-8) are obtained purely from geometry<sup>6</sup> with the assumption that the propagation speed  $w$  is constant.

We now turn our attention to the case of a material surface ( $w=0$ ) which is of great theoretical interest, and is the starting point for the development of the Stochastic Flamelet Model. With  $w=0$ , a "flamelet" becomes an infinitesimal material surface element, and  $\underline{X}(t)$  becomes the location of a fluid particle.

Since  $\dot{A}_R$  is zero (for  $w=0$ ), Eqs. (1), (7) and (8) can be integrated to determine the flamelet properties if  $\underline{U}(t)$  and  $U_{ij}(t)$  are known. Hence the first components of the model are stochastic models for these Lagrangian time series.

Space does not allow a full description of these models. Briefly  $\underline{U}(t)$  is simulated by a diffusion process<sup>15,16</sup> in which the diffusion coefficient depends on the dissipation  $\epsilon(t)$  following the fluid particle<sup>17</sup>. The logarithm of the dissipation is modelled as an Ornstein-Uhlenbeck stochastic process<sup>16</sup>. The velocity gradients are modelled as the product of  $\epsilon^{1/2}(t)$  and a linear combination of Gaussian stochastic processes. The linear combination is chosen so as to satisfy all constraints appropriate to homogeneous isotropic turbulence<sup>18</sup>. The coefficients in all these models are approximately matched to correlation functions (e.g.  $\langle U_{ij}(t+s)U_{kl}(t) \rangle$ ) obtained from direct numerical simulations<sup>19</sup> of isotropic turbulence at a Taylor-scale Reynolds number of about 40.

For the initially plane, infinite, material surface  $X_1(t_0) = 0$ , the surface-to-volume ratio  $\Sigma(\underline{x}, t)$  depends solely on  $x_1$  and  $t$ : initially it is  $\Sigma(x_1, t_0) = \delta(x_1)$ . The stochastic

model for  $\underline{U}(t)$  causes  $X_1(t)$  to disperse in accord with Taylor's theory<sup>20</sup>:  $X_1(t)$  is Gaussian with zero mean, and its standard deviation increases first linearly with time, but ultimately as  $\sqrt{t}$ . The stochastic model for the velocity gradients is independent of  $\underline{U}$  and  $\underline{X}$ , and hence so also is  $A(t)$ . Consequently, the profiles of  $\Sigma(x_1, t)$  have a Gaussian shape, their width increasing from zero first linearly with time, and later as  $\sqrt{t}$ .

The model for  $U_{ij}(t)$  correctly results in  $\langle \dot{A}(t) \rangle$  being zero initially; but after a few Kolmogorov time scales  $\langle A(t) \rangle$  increases exponentially with time in accord with Batchelor's supposition<sup>21</sup>. Hence the peak value  $\Sigma(0, t)$  — infinite initially — first decreases as the surface disperses (but stretches little), and then increases as stretching becomes dominant, eventually increasing as  $e^t/\sqrt{t}$ .

A flame sheet ( $w > 0$ ) differs in three ways from the material surface considered above: the flamelet does not follow a fluid particle; the density jump across the flame sheet influences  $\underline{U}$  and  $U_{ij}$  (through the associated pressure fields<sup>1</sup>); and, the term  $\dot{A}_R$  in Eq. (8) is non-zero. In this initial study we concentrate on the third effect — area reduction caused by propagation. We consider the constant-density case (thus eliminating the second effect), and use the models for  $\underline{U}$  and  $U_{ij}$  described above even for  $w > 0$ . (Direct numerical simulations are in progress to investigate the effect of non-zero  $w$  on these time series.) The flamelet motion (relative to the fluid) is correctly accounted for by Eq. (1).

Two mechanisms are responsible for the *area-reduction term*  $\dot{A}_R$ . Let  $H$  be the mean curvature of the surface, which is positive if the flame sheet is convex towards the reactants. Then one contribution to  $\dot{A}_R$  is  $6\dot{w}HA$ . The second contribution is due to cusps which can form either by the curvature becoming infinite, or by the flame-sheet propagating into itself. However caused, as cusps propagate, they tend to reduce the flame-sheet area<sup>4,9</sup> — leading to a positive contribution to  $\dot{A}_R$ .

We model both contributions together by

$$\dot{A}_R(t) = C_R w A(t) \Sigma(\underline{X}[t], t) \eta(t) / b(\underline{X}[t], t), \quad (9)$$



where  $C_R$  is a model constant,  $b(\underline{x}, t)$  is the mean volume fraction of reactants, and  $\eta(t)$  is an *orientation factor* defined below. This, we claim, is the simplest possible model that has the correct qualitative behavior. With the exception of the orientation factor it is the same as that proposed by Marble & Broadwell<sup>22</sup> in the context of turbulent diffusion flames.

One justification for the form of the model of  $\dot{A}_R$  (Eq. 9) is that it accurately describes the rate of area change of a diversity of geometrically simple surfaces. We cite three examples.

- i) Consider the (disconnected) flame-sheet consisting of many infinite, plane, parallel surfaces separated by slabs of reactants and products. If the thickness of the reactant slabs is uniformly distributed (in some finite interval) then the rate of area reduction is given by Eq. (9) with  $C_R \eta = \frac{1}{2}$ .
- ii) Consider the (disconnected) flame-sheet consisting of many equal-size spherical surfaces surrounding pockets of reactants. Then Eq. (9) with  $C_R \eta = \frac{2}{3}$  correctly gives the rate of area reduction. The same result (but with  $C_R \eta = \frac{1}{2}$ ) holds for circular cylindrical pockets of reactants.
- iii) Similar to ii), if the reactant pockets are equal-size regular polyhedra (e.g. cubes) then Eq. (9) holds again with  $C_R \eta = \frac{2}{3}$ , or for cylinders of regular polygonal cross-section we find  $C_R \eta = \frac{1}{2}$ .

While these examples bear little resemblance to the geometry of turbulent flame sheets, they nevertheless illustrate that different shapes and mechanisms lead to the same formula, i.e. Eq. (9). Note that in i) the area is reduced by the mutual annihilation of colliding flame sheets; in ii) the area reduction is solely due to curvature; and, in iii) it is solely due to cusps.

As well as arising automatically in the above examples, the factor  $b^{-1}$  in Eq. (9) is suggested by a realizability condition: in the statistically homogeneous case, as reaction nears completion,  $\Sigma$  and  $b$  must vanish together. If, as assumed,  $\dot{A}_R$  is linearly

proportional to  $\Sigma$ , then this realizability condition requires (as  $b$  tends to zero) that  $\dot{A}_R$  be proportional to  $b^{-1}$ . For the homogeneous case the model then predicts that  $\Sigma$  and  $b$  vanish together in finite time.

In the examples cited, the flame sheets are randomly orientated, and Eq. (9) holds with a constant value of  $C_R \eta$ . But the further example of a single, plane flame-sheet illustrates the need for the orientation factor  $\eta(t)$ . For this case there are no cusps or self-intersections, and the curvature is zero everywhere. Thus  $\dot{A}_R$  is zero. But it may be deduced (by a limiting process) that Eq. (9) (with  $C_R \eta$  being of order unity) implies that  $\dot{A}_R$  is infinite. This problem is remedied by introducing the orientation factor  $\eta(t)$ .

For the plane flame, a flamelet (with properties  $\underline{X}, A, \underline{N}$ ) has the same orientation as any other flamelet (with properties  $\underline{X}', A', \underline{N}'$ ). Thus  $\underline{N} \bullet \underline{N}'$  is unity. In general, if two flamelets (separated by a distance uniformly distributed in a finite interval  $L$ ) are on a collision course, then the probability of their colliding in the time interval  $dt$  is

$$dP = \sqrt{2} \, w \, dt \, (1 - \underline{N} \bullet \underline{N}')^{1/2} / L. \quad (10)$$

This follows from simple geometric considerations. For the case of a plane flame, the two flamelets collide at infinity and hence Eq. (10) correctly yields  $dP = 0$ , since  $\underline{N} \bullet \underline{N}'$  is unity.

In the Stochastic Flamelet Model, the orientation factor  $\eta(t)$  is based on the factor  $(1 - \underline{N} \bullet \underline{N}')^{1/2}$  appearing in Eq. (10). To be precise,  $\eta(t)$  is the conditional expectation of this factor, for  $\underline{N}'$  being any other flamelet at the same location (on a different realization):

$$\eta(t) \equiv \langle (1 - \underline{N}(t) \bullet \underline{N}'(t))^{1/2} \mid \underline{X}'(t) = \underline{X}(t) \rangle. \quad (11)$$

For the statistically isotropic case (randomly orientated flamelets) the orientation factor is unity.

We have described the area-reduction model as a deterministic process: at the rate  $\dot{A}_R$ , the flamelet's area decreases smoothly and deterministically. This is the appropriate physical model if the area reduction is due to curvature. Alternatively the model could be

implemented as a stochastic point process: in the time interval  $dt$ , with probability  $\dot{A}_R dt$ , the flamelet is annihilated (i.e.  $A(t+dt)=0$ ), while with probability  $1-\dot{A}_R dt$  the flamelet area is unchanged. This is the appropriate physical model if the area reduction is due to cusps. As far as single-time statistics are concerned, the result is the same however the model is implemented. The deterministic implementation is chosen since it results in smaller statistical errors in the Monte Carlo solution algorithm.

To summarize the model: stochastic processes are used to simulate the velocity  $\underline{U}(t)$  and its derivative  $U_{ij}(t)$  following the flamelet. Equations (1) and (7) are integrated to determine the position  $\underline{X}(t)$  and orientation  $\underline{N}(t)$  of the flamelet, while the area amplification  $A(t)$  is obtained by integrating Eq. (8). The first term in Eq. (8), on average, causes an area increase, while the second is an area reduction due to curvature, cusps and self-intersections. This area reduction term is given by Eqs. (9) and (11). From the flamelet properties the surface-to-volume ratio  $\Sigma(\underline{x},t)$  can be determined (Eq. 4), and hence the local burning rate  $\omega(\underline{x},t)$  (Eq. 6) is obtained.

We have described the model for a single representative flamelet. To implement the model numerically we consider an ensemble of  $N_f \approx 13,000$  such flamelets. The expectations — such as are required to determine  $\Sigma(\underline{x},t)$  — are approximated by ensemble averages.

The burning rate  $\omega(\underline{x},t)$  obtained from the flamelet model is used in the solution of the modelled transport equation<sup>15</sup> for the joint pdf of velocity, dissipation, and reaction progress variable,  $c$ . The Monte Carlo solution of the joint pdf equation amounts to simulating the evolution of velocity, dissipation and  $c$  of an ensemble of  $N_p \approx 35,000$  fluid particles. For velocity and dissipation, exactly the same stochastic models are used as for the flamelets. At  $(\underline{x},t)$ , the mean rate at which reactants ( $c=0$ ) burn (i.e. change to  $c=1$ ) is simply  $\omega(\underline{x},t)$ . From the joint pdf calculation, the mean volume fraction of reactants  $b(\underline{x},t) = 1 - \langle c(\underline{x},t) \rangle$  is obtained and supplied to the Stochastic Flamelet Model.

## RESULTS

The Stochastic Flamelet Model in combination with the joint pdf method has been used to simulate the idealized case of an initially plane flame. The flow is statistically-stationary, homogeneous, isotropic turbulence with zero mean velocity. The turbulent kinetic energy  $k$  and the mean dissipation rate  $\langle \epsilon \rangle$  are taken to be unity: hence the turbulence intensity is  $u' = \sqrt{2/3}$ . The Taylor-scale Reynolds number is 40, and the Kolmogorov time scale is 0.064.

At the initial time ( $t=t_0=0$ ) a plane flame sheet at  $x_1=0$  separates reactants ( $c=0, x_1>0$ ) from products ( $c=1, x_1<0$ ). We investigated two laminar flame speeds:  $w=0.01$  and  $w=1.0$  (or  $w/u' = 0.0122$  and  $w/u' = 1.22$ ).

For the smaller laminar flame speed ( $w=0.01$ ) Fig. 2 shows the total flame sheet area  $A_T$  (per unit initial area) as a function of time. It may be seen that for large times ( $t>2$ , say)  $A_T$  asymptotes to a value of about 300. At these times the area generation by stretching (the first term in Eq. 8) is balanced by the area reduction  $\dot{A}_R$ . But at early times ( $t<0.5$ , say), because  $w\Sigma$  is small,  $\dot{A}_R$  is small. Thus the flame sheet behaves much like a material surface: after a small transient ( $0 \leq t \leq 0.1$ , say),  $A_T$  increases exponentially with time.

Figure 3 shows the loci of the constant concentration points in the flame:  $x_\alpha(t)$  is defined such that

$$\langle c(x_1 = x_\alpha[t], t) \rangle = \alpha. \quad (12)$$

Thus  $x_{0.5}(t)$  is the locus of the center of the flame, and  $x_{0.1}(t)$  and  $x_{0.9}(t)$  are taken to mark the front and back of the flame, respectively.

It may be seen that initially ( $t<0.5$ , say) the flame barely moves ( $x_{0.5} \approx 0$ ), and its width  $x_{0.1}-x_{0.9}$  grows linearly in time. Again, this is because the slowly propagating flame sheet behaves (initially) like a material surface: there is little combustion. But as time progresses and  $A_T$  grows, burning becomes significant, and the flame begins to move. At

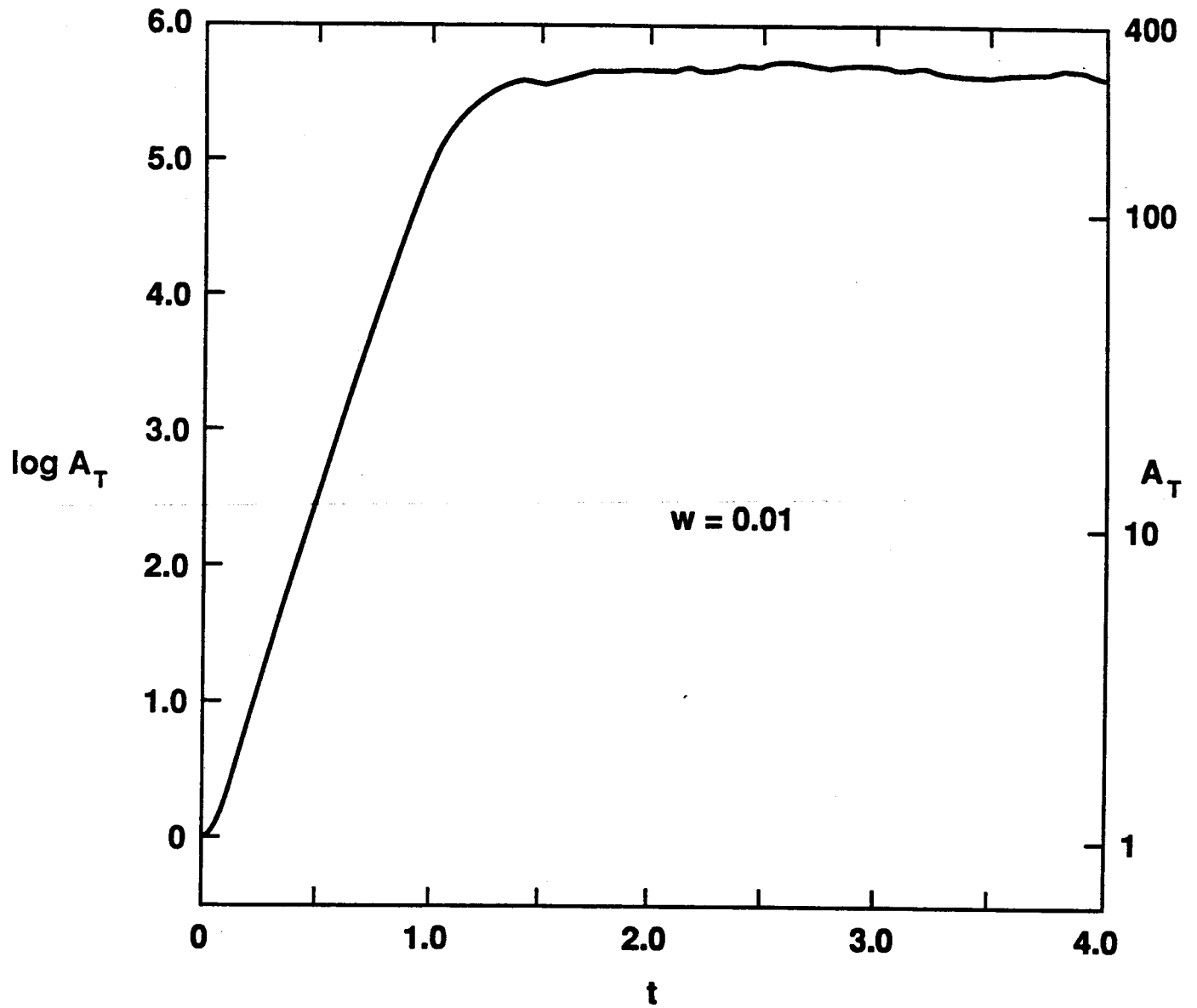


Figure 2: Natural Logarithm of Flame Sheet Area (Per Initial Area) Against Time. Propagation Speed  $w=0.01$ .

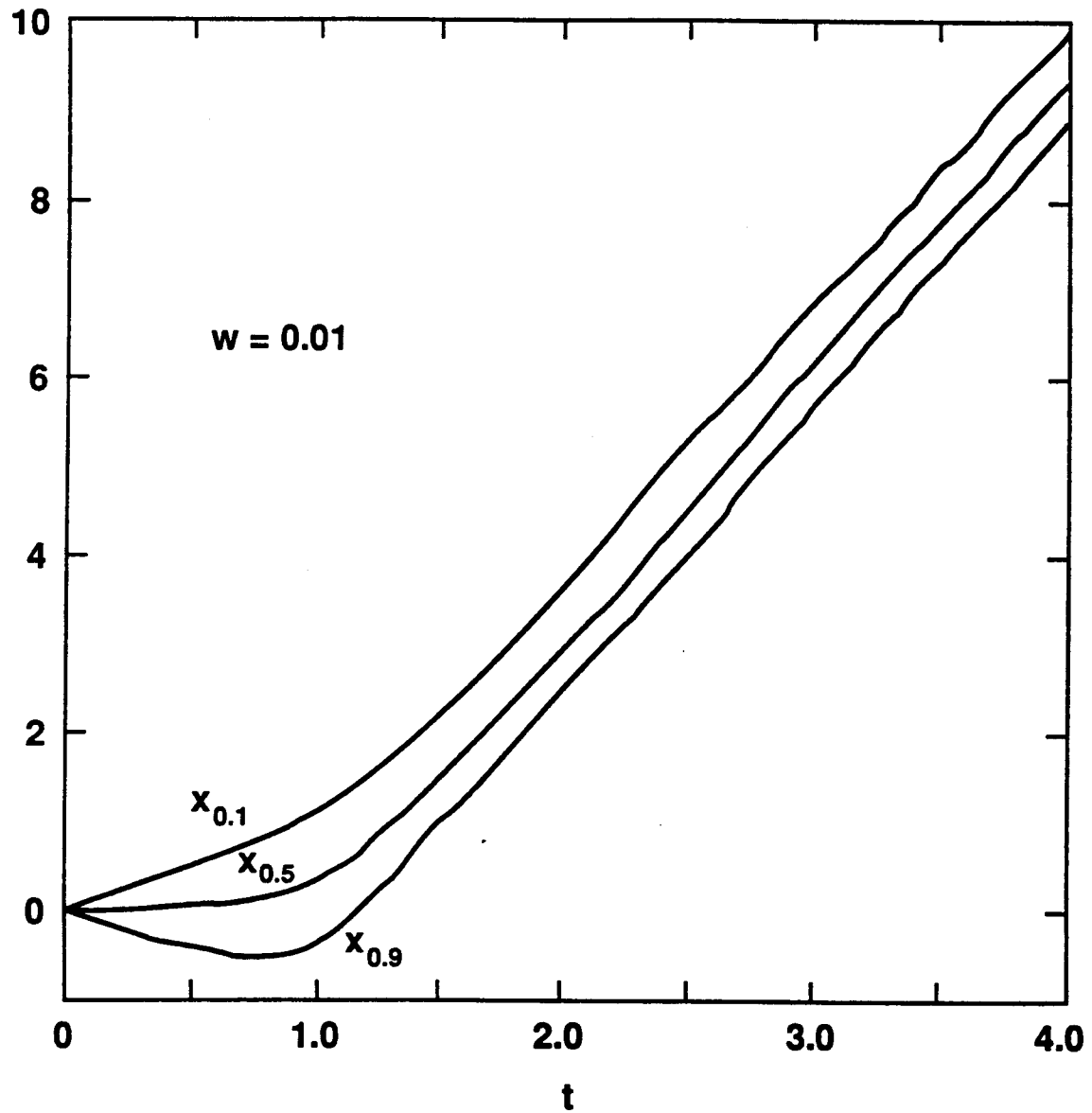


Figure 3: Loci of Points  $x_{0.1}(t)$ ,  $x_{0.5}(t)$ ,  $x_{0.9}(t)$  at Which the Mean Progress Variable is 0.1, 0.5 and 0.9 Respectively. Propagations Speed  $w=0.01$ .

large times ( $t > 2$ , say) the turbulent flame speed  $u_T = dx_{0.5}/dt$  (or  $wA_T$ ) adopts a constant value of about 3.0, and the constant width  $x_{0.1}-x_{0.9}$  is about 1.2.

The same plots for the fast laminar flame speed ( $w=1.0$ ) are shown on Figs. 4 and 5. Initially  $A_T$  decreases to a minimum of 0.95, then increases rapidly, and more slowly asymptotes to a value of 3.4. The initial decrease is physically impossible and is a defect — perhaps a small one — in the model. Even with the inclusion of the orientation factor,  $\eta(t)$ , at small (non-zero) times an initially plane flame develops positive area reduction  $\dot{A}_R$  faster than it is stretched by the turbulence.

In contrast to the case  $w=0.01$ , Fig. 5 shows that with  $w=1.0$ , significant burning starts immediately. The asymptotic value of the turbulent flame speed  $u_T$  is 3.4, while the thickness is again about 1.2.

An interesting statistic is  $\langle N_1(t) \rangle$  — the component of the normal in the  $x_1$ -direction, averaged over the flame sheet. Initially it is unity. For the slow flame speed ( $w=0.01$ ), and for a material surface ( $w=0$ ), after about one time unit  $\langle N_1 \rangle$  asymptotes to zero as the flamelets loose memory of their initial orientation. But for the faster flame speed ( $w=1.0$ ) the asymptotic value is 0.32. This is because flamelets moving backwards (negative  $N_1$ ) or sideways ( $N_1 = 0$ ) suffer greater area reduction than those moving forward ( $N_1 > 0$ ).

Figure 6 shows profiles of the mean reaction progress variable  $\langle c(x_1, t) \rangle$ , and the surface-to-volume ratio  $\Sigma(x_1, t)$ , in the asymptotic state of the flame with  $w=1.0$ . (For the flame with  $w=0.01$  the shapes of the profiles are similar, but  $\Sigma$  is larger by a factor of about 100.) The profile shapes are quite different at the front and back of the flame. At the front both  $\Sigma$  and  $\langle c \rangle$  have long tails, while at the back  $\Sigma$  and  $b (=1-\langle c \rangle)$  vanish quite abruptly. At the front, because  $b$  is small, area reduction is small, and the flame area grows by turbulent straining. Towards the center of the flame, as  $b$  becomes significant, area reduction begins to dominate causing  $\Sigma$  to decrease.

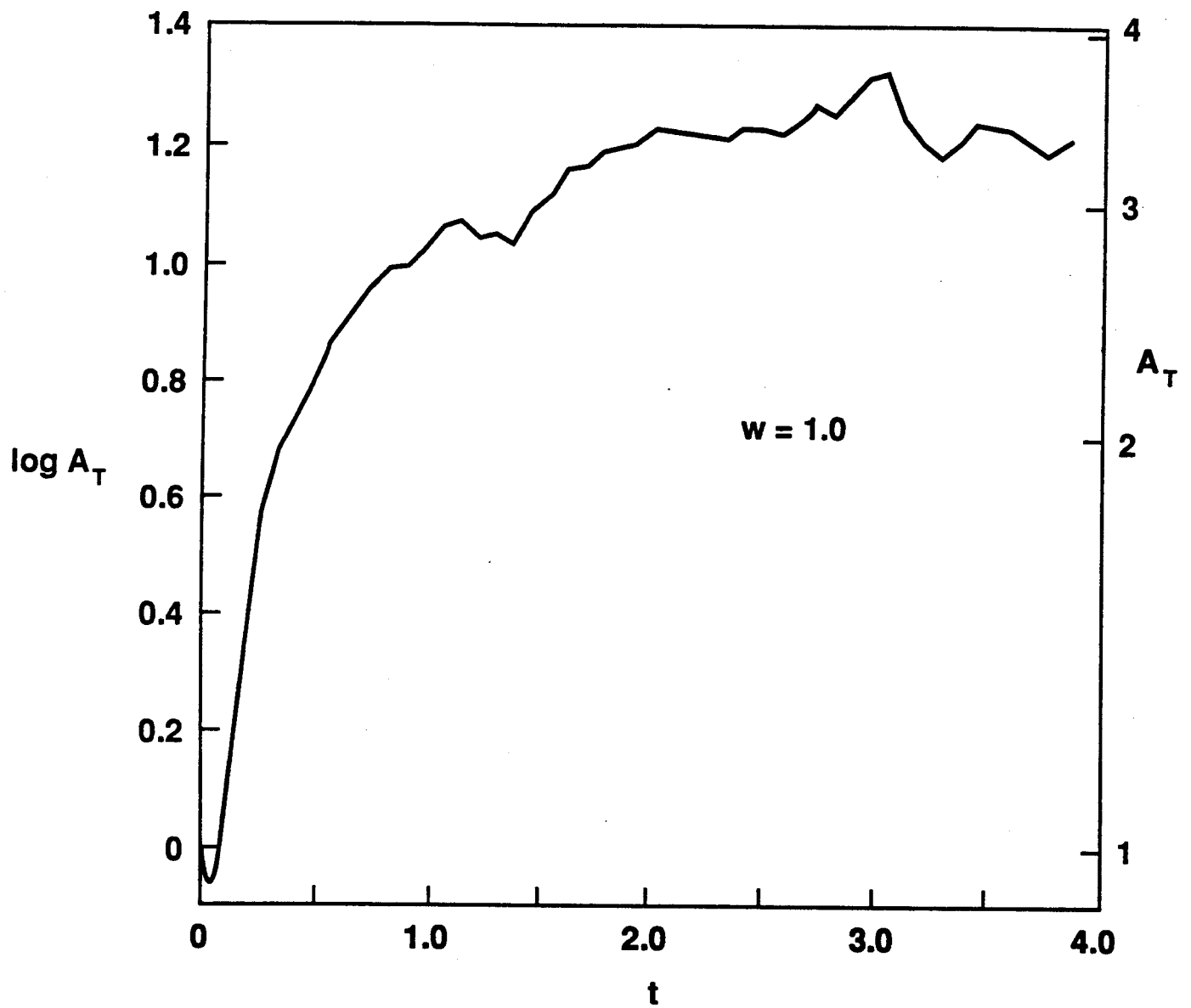


Figure 4: Natural Logarithm of Flame Sheet Area (Per Initial Area) Against Time. Propagation Speed  $w=1.0$ .



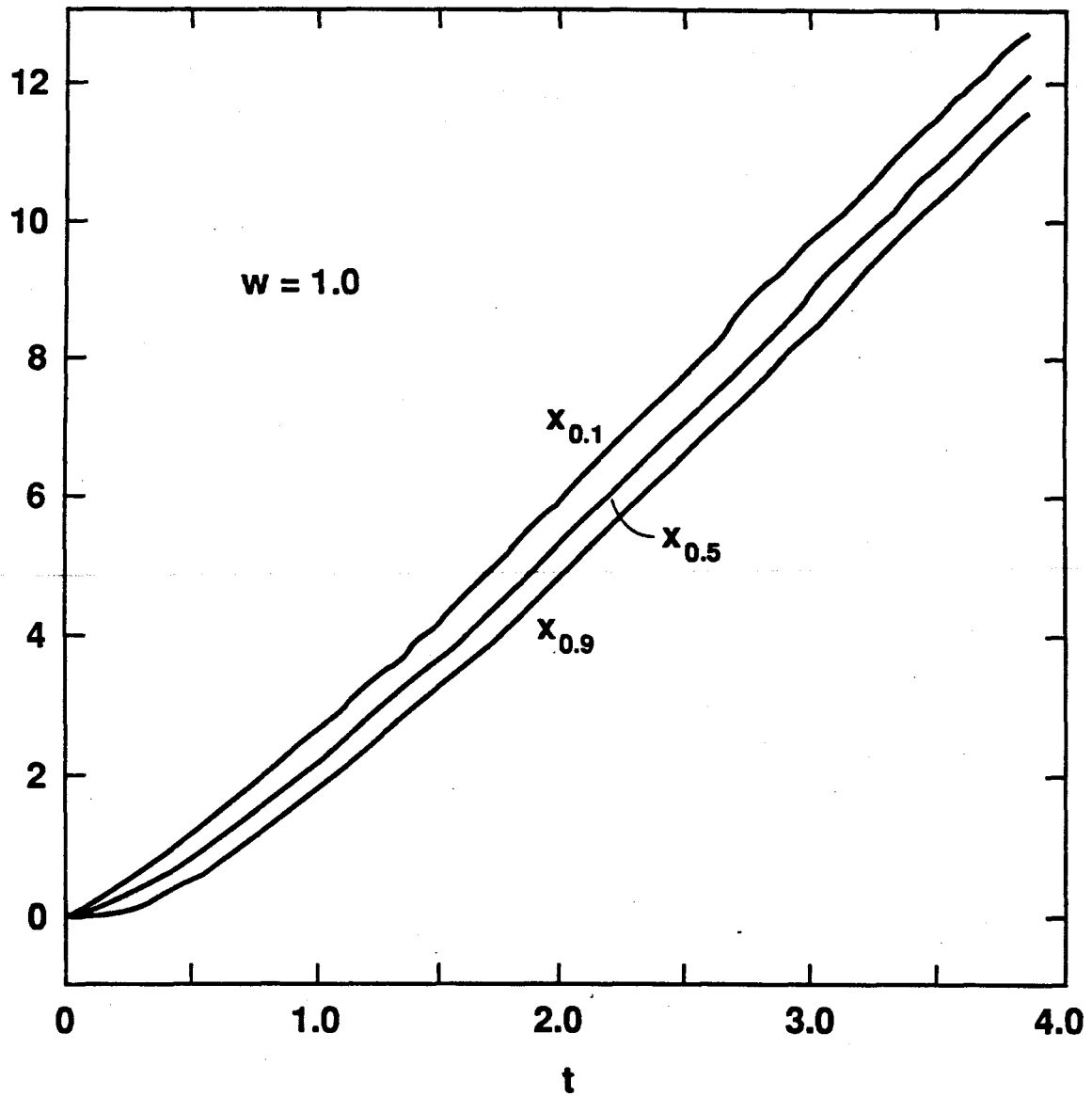


Figure 5: Loci of Points  $x_{0.1}(t)$ ,  $x_{0.5}(t)$ ,  $x_{0.9}(t)$  at Which the Mean Progress Variable is 0.1, 0.5 and 0.9 respectively. Propagations Speed  $w=1.0$ .

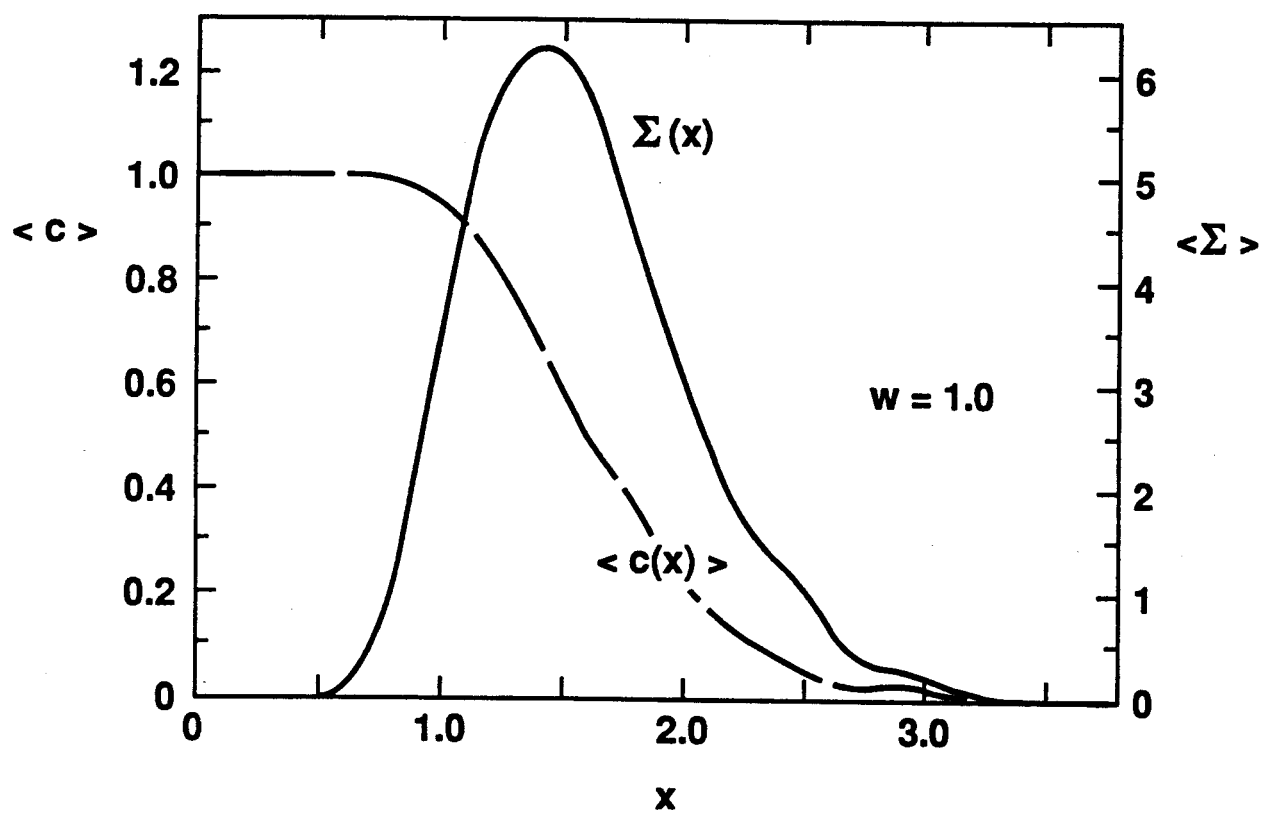


Figure 6: Profiles of Mean Progress Variable and Surface-to-Volume Ratio. (The Origin of  $x$  has been Shifted.)

## DISCUSSION AND CONCLUSIONS

In this work we have described and demonstrated the Stochastic Flamelet Model for turbulent premixed flames in the flamelet regime. The sample Monte Carlo calculations presented in the previous section, confirm that the model and numerical algorithm provide a tractable calculation procedure for non-stationary, inhomogeneous flames. Each of the calculations reported required about 150 CPU minutes on a minicomputer which is equivalent to 2 CPU minutes on a CRAY XMP.

As mentioned in the Introduction, existing models — the Bray-Moss-Libby model<sup>10,11</sup>, or the joint pdf method<sup>12-15</sup>, for example — have difficulty in determining the local rate of burning. Perhaps this is inevitable, since these models contain no information about the flame sheet that is responsible for the fuel consumption. The Stochastic Flamelet Model, on the other hand, contains a rather natural and complete statistical description of the flame sheet — its position, orientation and area. Because of this, the essential physical processes are readily incorporated in a natural manner. Most important among these are the straining of the flame sheet, the influence of the laminar flame speed, and the area reduction caused by curvature and cusps.

This first effort leaves many improvements and extensions ahead. The models of velocity  $\underline{U}(t)$  and its gradient  $U_{ij}(t)$  following a flamelet require further development and validation, in particular with regard to their dependence on Reynolds number and the laminar flame speed. Direct numerical simulations will provide invaluable information for this purpose.

The essential extension of the model to the variable-density case holds both difficulty and promise. The principal difficulty is that the velocity field — especially in the vicinity of the flame sheet — is affected by the flame sheet's propagation. Hence  $\underline{U}$  and  $U_{ij}$  are no longer purely turbulence quantities, but are directly affected by the flame sheet itself. Modelling aside, there is no difficulty in extending the calculation procedure to

variable-density flow: indeed previous pdf calculations of premixed flames<sup>13,14</sup> have incorporated realistic density ratios.

The promise is that the additional information contained in the flamelet model may lead to improvements in the modelling of the effect of combustion on the turbulence. A major uncertainty in both the Bray-Moss-Libby model<sup>10,11</sup> and the joint pdf method<sup>14</sup> is that the pressure fluctuations due to combustion are ignored. As observed by Pope<sup>1</sup>, some of these pressure effects can be directly related to flame-sheet processes.

#### NOMENCLATURE

- $A(t)$  - flamelet area amplification factor
- $A_0$  - initial expected surface area
- $\dot{A}_R$  - rate of area reduction due to cusps and curvature
- $A_s(t)$  - total expected surface area
- $A_T$  - total expected surface area per unit initial area
- $A_v$  - flamelet area within volume  $V$
- $b(\underline{x}, t)$  - mean volume fraction of reactants
- $C_R$  - model constant for area reduction
- $c(\underline{x}, t)$  - reaction progress variable
- $dA(t)$  - flamelet area
- $dA_0$  - initial flamelet area
- $H$  - mean curvature
- $\underline{N}(t)$  - unit normal vector into reactants
- $S_0$  - initial surface
- $t$  - time
- $t_0$  - initial time
- $\underline{U}(t)$  - velocity of a flamelet
- $U_{i,j}(t)$  - velocity derivative  $\partial u_i / \partial x_j$  following a flamelet

- $V$  - volume  
 $\underline{u}(\underline{x},t)$  - Eulerian fluid velocity field  
 $w$  - surface propagation speed (here equals laminar flame speed)  
 $\underline{X}(t)$  - flamelet position  
 $\underline{X}_0$  - initial flamelet position  
 $\underline{x}$  - position (independent variable)  
 $\delta(\underline{x})$  - three-dimensional Dirac delta function at  $\underline{x}$   
 $\epsilon(t)$  - dissipation rate  
 $\eta(t)$  - orientation factor  
 $\Sigma(\underline{x},t)$  - surface to volume ratio  
 $\omega(\underline{x},t)$  - local mean burning rate (volume burnt per unit volume per unit time)  
 $\langle \rangle$  - mean

## ACKNOWLEDGMENTS

This work was supported by the Department of Energy under contract number DE-ACS 02-83ER 13038, Dr. Oscar Manley contract manager. The Direct Numerical Simulations<sup>19</sup> used in the model development were supported by the Air-Force Office of Scientific Research (Grant number AFOSF-85-0083), and were performed at the Cornell National Supercomputer Facility which is supported in part by the National Science Foundation, New York State and IBM Corporation.

## REFERENCES

1. Pope, S.B.: Ann. Rev. Fluid Mech. 19, 237 (1987).
2. Abraham, J., Williams, F.A. and Bracco, F.V.: SAE paper 850345 (1985).
3. Bray, K.N.C.: in Turbulent Reactive Flows, ed. Libby, P.A. and Williams, F.A., Springer-Verlag, 1980.
4. Karlovitz, B., Denniston, D.W. Jr., Knappschaefer, D.H. and Wells, F.E.: Fourth Symposium (International) on Combustion, p. 613, Williams and Wilkins, Baltimore, 1953.

5. Markstein, G.M.: Non-Steady Flame Propagation, Macmillan, New York, 1964.
6. Pope, S.B.: The Evolution of Surfaces in Turbulence, Int. J. Eng'ng. Sci. (1988), in press.
7. Tabaczynski, R.J., Trinker, F.H. and Shannon, A.S.: Combust. Flame, 39, 111 (1980).
8. Clavin, P. and Williams, F.A.: J. Fluid Mech. 90, 589 (1979).
9. Thomas, A.: Combust. Flame, 65, 291 (1986).
10. Bray, K.N.C. and Moss, J.B.: Acta Astronautical 4, 291 (1977).
11. Libby, P.A.: Prog. Energy Combust. Sci. 11, 83 (1985).
12. Pope, S.B. and Anand, M.S.: Twentieth Symposium (International) on Combustion, p. 403, Combustion Institute, Pittsburgh, 1984.
13. Pope, S.B. and Cheng, W.K.: Twenty-First Symposium (International) on Combustion, p. 1473, Combustion Institute, Pittsburgh, 1986.
14. Anand, M.S. and Pope, S.B.: Combust. Flame 67, 127 (1987).
15. Pope, S.B.: Prog. Energy Combust. Sci. 11, 119 (1985).
16. Karlin, S. and Taylor, H.M.: A Second Course in Stochastic Processes, Academic, New York, 1981.
17. Pope, S.B. and Chen, Y-L.: Bull. Amer. Phys. Soc. 31, 1734 (1986).
18. Hinze, J.O.: Turbulence, McGraw Hill, New York, 2nd. Ed., 1979.
19. Yeung, P.K., Girimaji, S. and Pope, S.B.: Eulerian and Lagrangian Statistics from a High-Resolution Direct Simulation of Stationary Homogeneous Turbulence, Cornell University Report, FDA-88-02, 1988.
20. Taylor, G.I.: Proc. London Math. Soc. 20, 196 (1921).
21. Batchelor, G.K.: Proc. Roy. Soc. A 213, 349 (1952).
22. Marble, F.E. and Broadwell, J.E.: The Coherent Flame Model of Turbulent Chemical Reactions, TRW Report, 1977.