NUMERICAL MODELING OF TURBULENT COMBUSTION

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Our work in numerical modeling is focused on the use of the random vortex method to treat turbulent flow fields associated with combustion while flame fronts are considered as interfaces between reactants and products, propagating with the flow and at the same time advancing in the direction normal to themselves at a prescribed burning speed. The latter is associated with the generation of specific volume (the flame front acting, in effect, as the locus of volumetric sources) to account for the expansion of the flow field due to the exothermicity of the combustion process. The model was applied to the flow in a channel equipped with a rearward facing step. The results we obtained revealed the mechanism of the formation of large scale turbulent structure in the wake of the step, while it showed the flame to stabilize on the outer edges of these eddies(1).

In the course of this year we concentrated upon three topics:

1. Study of the fundamental aspects of the modeling technique
2. Application of the model to the formation of a turbulent jet
3. Development of novel concepts bringing forth the aerodynamic properties of turbulent flames

On the first subject, three efforts have been successfully pursued. First is the development of the random element method, presenting the application of the random walk technique to model diffusion of energy. The concept of vortex sheets and vortex blobs is extended for this purpose to heat transfer sheets or temperature jump elements, and blobs of internal energy, that carry thermal gradients from heat conducting walls to the interior of the field and redistribute them by diffusion. Table 1 presents the fundmental idea of random walk modeling of diffusion, exploiting the analogy between the Green junction of the diffusion equation and the probability density junction of a Gaussian random variable. Figures 1 and 2 show a comparison between the exact solution and the numerical solution for the problem of heating an infinite solid by an isothermal wall at $y = 0$, in terms of the heat flux profiles and the temperature profiles. Figures 3 and 4 depict the temperature profiles for a finite solid bounded by two isothermal walls, and an isothermal and an adiabatic wall, respectively. The extention of the procedure to handle two-dimensional diffusion is presented in Table 2. A one-dimensional approximation close to the walls is employed to implement isothermal boundary conditions, while energy elements are used in the interior to diffuse the energy there. Figures 5 and 6 display the temperature profiles along the diagonal of a corner and a square, respectively, as compared to the corresponding exact profiles.

The second fundmental problem we have solved is concerned with the generation of vorticity by the interaction between the pressure field and density gradients -- a mechanism which is of importance to both flames and buoyancy effects. The motion of the temperature jump elements, governed by the algorithm of the random element method, generates elements of vorticity in the interior of the field while additional elements are generated by the no-slip condition at the walls. Table 3 describes how random walk is used in conjunction with the principle of time splitting to solve the system of equations that describes natural convection flow over a vertical infinite isothermal wall. Figure 7 shows a comparison between our solution (thick lines) and a finite difference solution for two values of the Prandtl number[3].

The third problem in this category is that of flame propagation. In our original model an interface advection and propagation algorithm, based on the assumption that the flame is a jump in density, was used to propagate the flame. In order to treat flame propagation as that of a reacting surface governed by a finite rate of reaction, the problem was recast in terms of a reaction-diffusion equation in temperature. The algorithm of the random element method was extended to solve this problem by adjusting the strength of the temperature jump elements as they move according to the rate of reaction as described in Table 4.

The algorithm was tested by solving problems by the use of finite difference and finite element methods, demonstrating its capability of calculating flame propagation with proper accuracy. Figures 8 and 9 show a comparison between the exact solution, evaluated for $f(T) = T(1-T)$, and the numerical computations when the integration of the reaction part of the equation is done using a first-order Euler scheme in the first case, and an exact integral in the second case, respectively[4].

On the second subject, the random vortex method was applied to the problem of the formation of planar, two-dimensional turbulent jet at high Reynolds numbers. Figure 10 describes schematically the elementary processes of the random vortex method and how they are implemented to solve the convection-diffusion equation. The results, expressed in terms of the development of the vorticity field, are presented in Fig. 11. They reveal the formation of large scale turbulent eddy structures on both sides of the jet with a potential core inside. Few jet widths downstream , the two layers start to interact and the flow becomes dominated by the pairing of eddies from both sides. The turbulent eddies grow by entraining the non-turbulent fluid, while their trajectories become more and more convoluted as a result of the interaction between positive and negative vorticity. These pictures display a remarkable resemblence to experimental photographs obtained by Dimotakis, et al. [5] across the plane of symmetry of an exisymmetric jet.

The concept of flame aerodynamics has been developed on the basis of our numerical modeling studies, supported by experimental observations of turbulent flames. The ultimate conclusion of these studies is the dominance of large scale eddies over the flow field, while the flame itself becomes established at the outer edges of these eddies and acts as a semi-permeable membrane encompassing the burnt gases. It is the interaction between these eddies and the expansion associated with the exothermicity of combustion process that produces the characteristic aerodynamic pattern that we are now studying[6].

REFERENCES

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TABLE 1. FUNDAMENTAL IDEA

Differential Equation	$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial y^2}$
Boundary Conditions	$\phi(y,0) = \delta(0)$; $\phi(\pm \infty,t) = 0$
Constraint	$\Phi = \int_{-\infty}^{\infty} \phi \, dy = 1$
Formal Solution	$\phi = \frac{1}{\sqrt{2\pi}\sigma} \exp[-(y/\sigma)^2]$; $\sigma = \sqrt{2\alpha t}$
Stochastic Solution	$\Sigma \delta\Phi_i = 1$ $y_i(t + \Delta t) = y_i(t) + \eta_i$ $E(\eta_i) = 0$; $E(\eta_i^2) = 2\alpha \Delta t$
Local Sampling	$\phi = \frac{1}{\delta y} \Sigma \delta\Phi_i \delta(y-y_i)$
Global Sampling	$\Phi = \Sigma \delta \Phi_i H(y-y_i)$

Nomenclature

H - Heavyside step function

δ - Dirac delta function

E - Expected value

η - Gaussian random variable

σ - Standard deviation

TABLE 2. A HYBRID SCHEME FOR TWO-DIMENSIONS

DOMAIN	BOUNDARY $y < \delta_s$	INTERIOR $y > \delta_s$
Differential Equation	$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial y^2}$	$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$
Boundary Condition	$T = 1$	$T = \delta(y-\delta_s)$
Diffusing Element	δT_i	δe_i
Coupling	$\delta e_i = \delta T_i * (y_i - \delta_s)$	$\delta T_i = \pm \delta e_i / \delta_s$
Stochastic Solution	$\underline{r}_i(t+\Delta t) = \underline{r}_i(t) + \eta_i$	$\underline{r}_i(t+\Delta t) = \underline{r}_i(t) + \underline{\eta}_i$
Sampling	$T = \frac{\Sigma\ \delta e_i}{\delta_s \cdot dx} + \Sigma\ \delta T_i H(y-y_i)$	$T = \frac{1}{\delta A_i} \Sigma\ \delta e_i\ \delta(\underline{r}-\underline{r}_i)$

$\delta_2 = 2\sigma$; thickness of 1-D diffusion layer

δA_i = area element

TABLE 3. PRESSURE-DENSITY INTERACTION

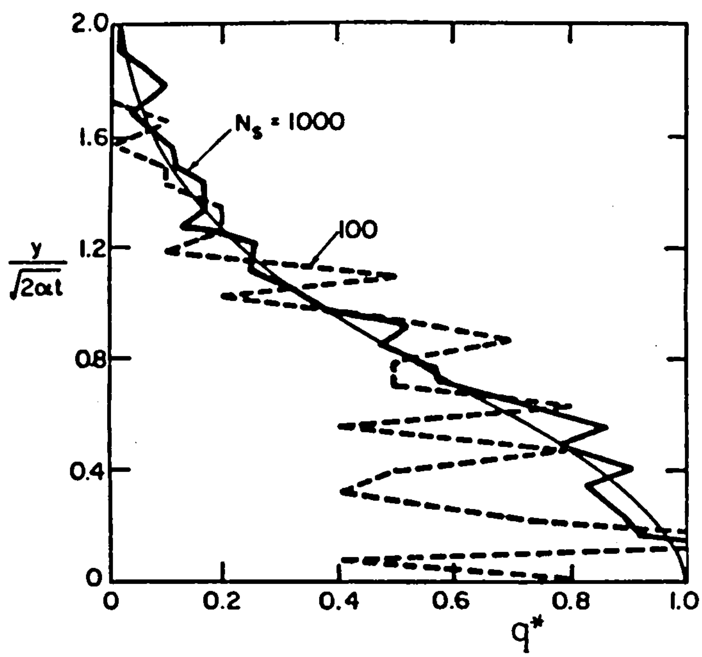
DIFFERENTIAL EQUATIONS	$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$ $\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} + g\beta\,(T-T_\infty)$
INITIAL CONDITIONS	$T = 0 \;;\; u = 0$
BOUNDARY CONDITIONS	$x = 0 \quad T = 1 \;;\; u = 0$ $x = \infty \quad T = 0 \;;\; u = 0$
FRACTIONAL STEPS	$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \;;\; \frac{\partial \xi}{\partial t} = \nu \frac{\partial^2 \xi}{\partial x^2}$ $\frac{\partial \xi}{\partial t} = g\beta \frac{\partial T}{\partial x}$
VORTICITY PRODUCTION	$\delta\gamma = g\beta\,\delta T$ $T = \sum_n \delta T\, H(x-x_i)$ $\gamma = \sum_N \delta\gamma\, H(x-x_i)$ $N(t+\Delta t) = N(t) + 2n$

n = number of temperature jump elements

N = Number of vortex elements

TABLE 4. REACTION-DIFFUSION EQUATION

DIFFERENTIAL EQUATION	$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + f(T)$
INITIAL CONDITION	$T(x,0) = T_0(x)$
BOUNDARY CONDITIONS	$T(+\infty,0) = 0 \quad ; \quad T(-\infty,0) = 1$
SOLUTION	
FRACTIONAL STEPS	$T(n\Delta t) = [R(\Delta t)\ D(\Delta t)]^n\ T_0$
REACTION	$\frac{dT}{dt} = f(T)$
DIFFUSION	$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$
DETERMINISTIC	$\delta T_i(t + \Delta t) = \delta T_i(t) + f(T_i)\ \Delta t$
STOCHASTIC	$T = \sum \delta T_i\ H(x-x_i)$ $x_i(t + \Delta t) = x_i(t) + \eta_i$ $E[\eta] = 0 \quad ; \quad E[\eta^2] = 2\ \Delta t$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1.2
0.8
0.4
0
$\frac{y}{\sqrt{2\alpha t}}$
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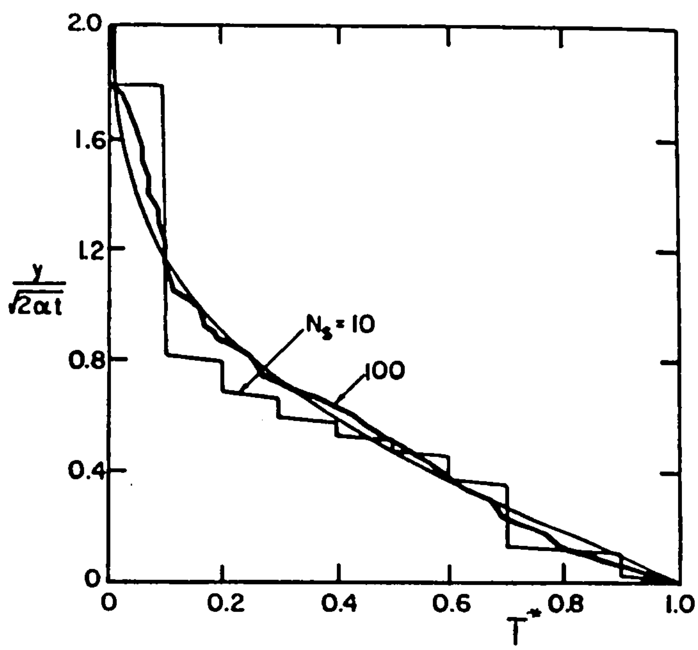
0
0.2
0.4
0.6
0.8
1.0
q^*

Fig. 1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0.8
0.4
0
$\frac{y}{\sqrt{2\alpha t}}$
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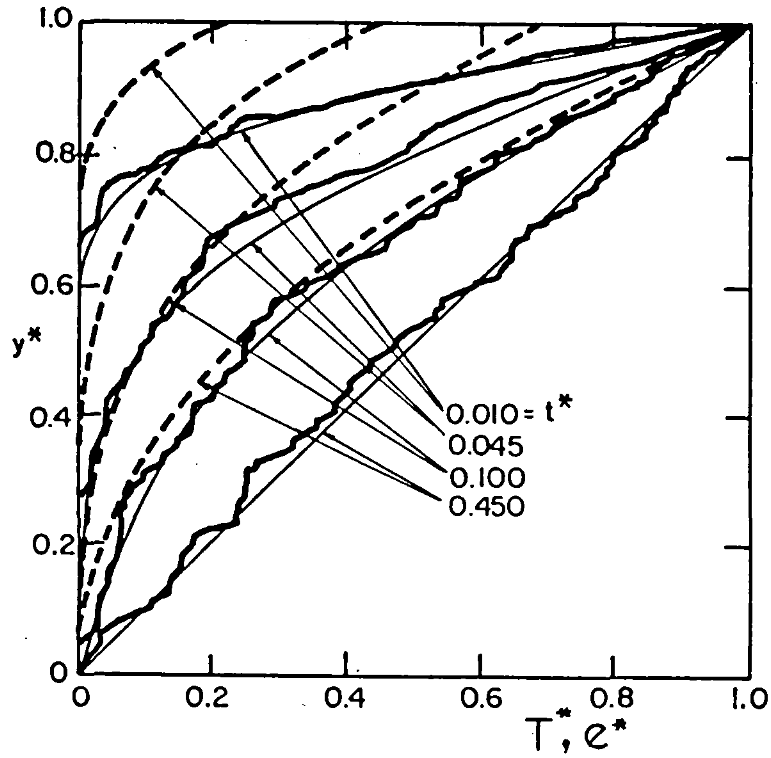
0.2
0.4
0.6
0.8
1.0
T^*

Fig. 2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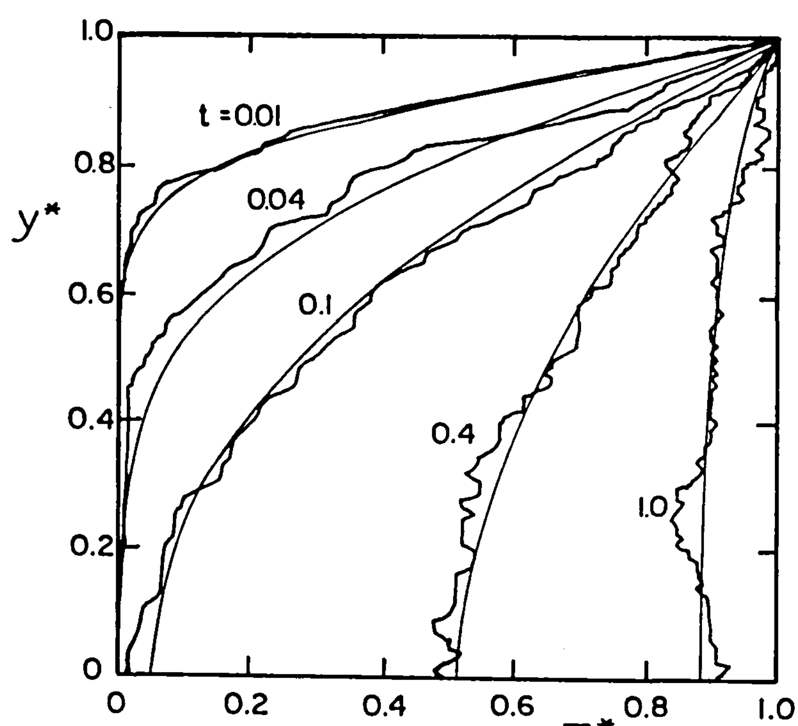
0.8
0.6
y*
0.4
0.2
0
0.010 = t*
0.045
0.100
0.450
0
0.2
0.4
0.6
0.8
1.0
T*, e*

Fig. 3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0.8
y*
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0.4
0.2
0
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0.4
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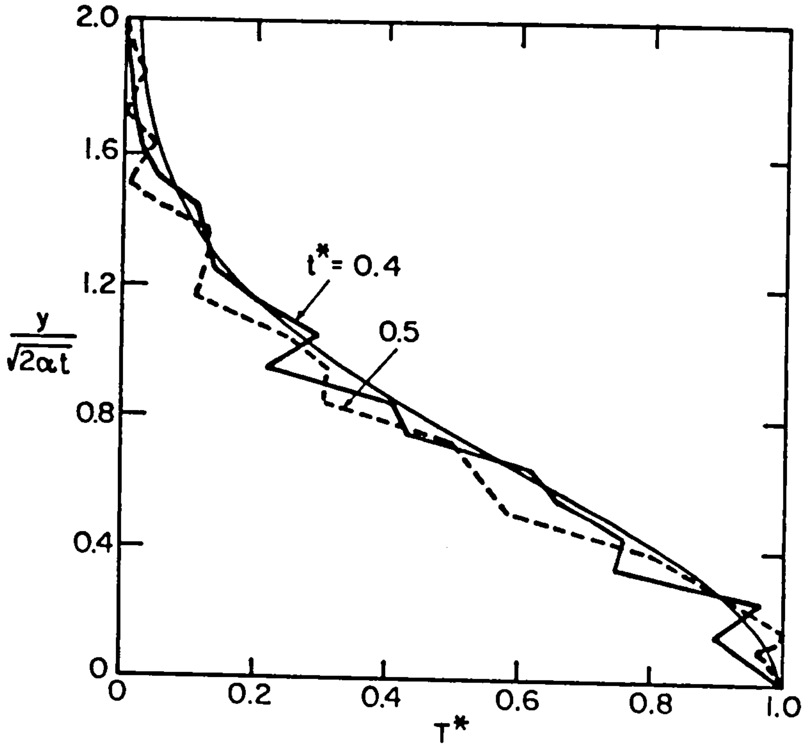
0.8
1.0
T*

Fig. 4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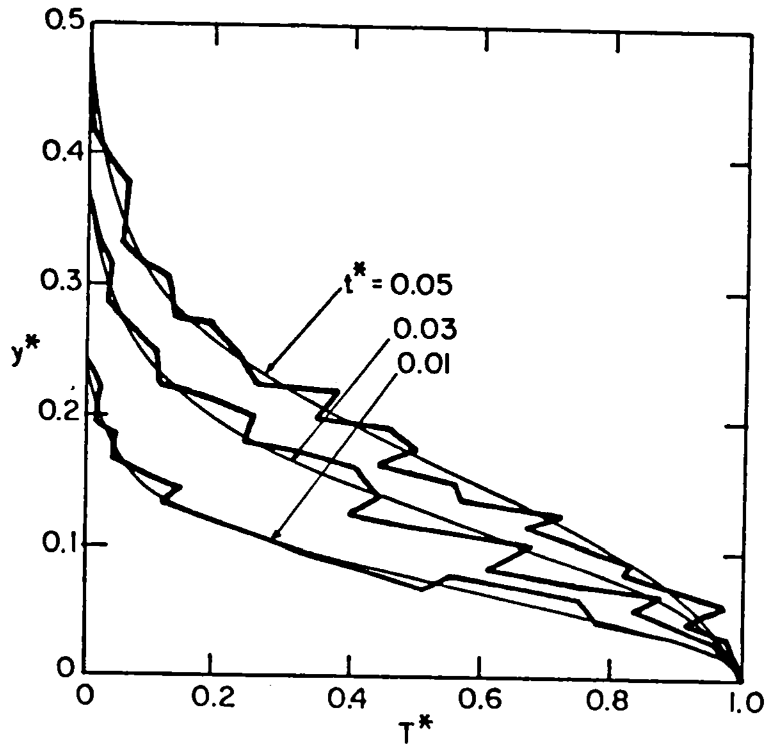
1.6
1.2
0.8
0.4
0
y/√2αt
0
0.2
0.4
0.6
0.8
1.0
T*
t* = 0.4
0.5

Fig. 5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0.4
0.3
0.2
0.1
0
y*
0
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0.4
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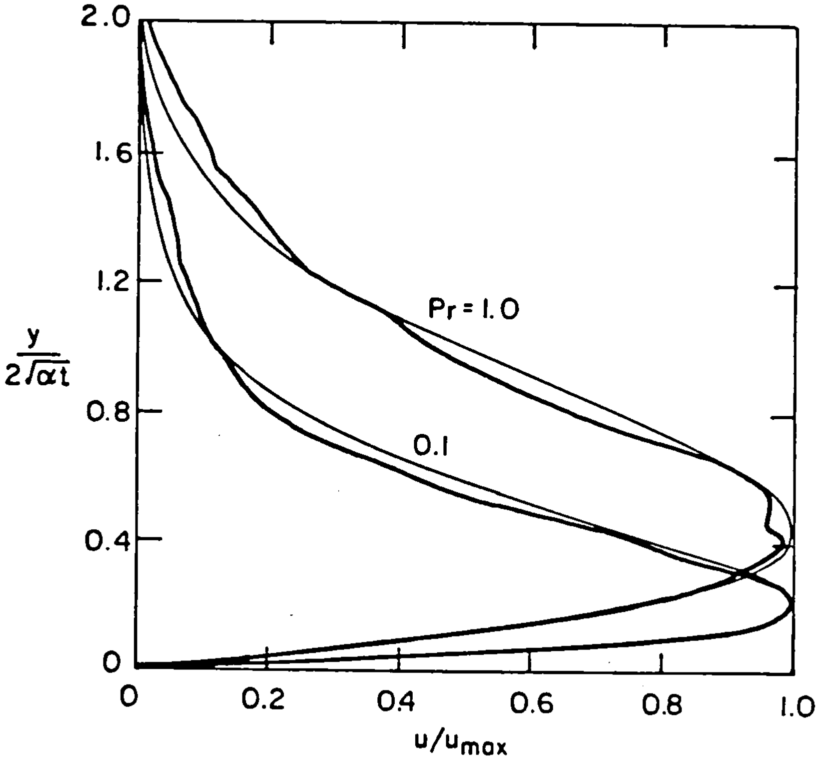
0.8
1.0
T*
t* = 0.05
0.03
0.01

Fig. 6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1.6
1.2
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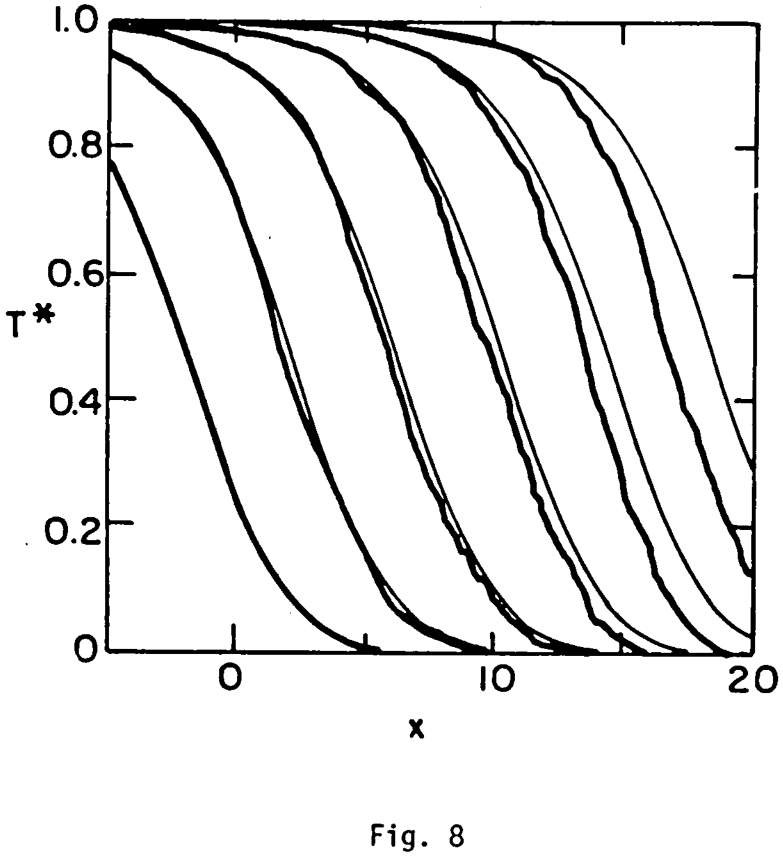
0.4
0
0
0.2
0.4
0.6
0.8
1.0
u/u_max
Pr = 1.0
0.1

Fig. 7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T*
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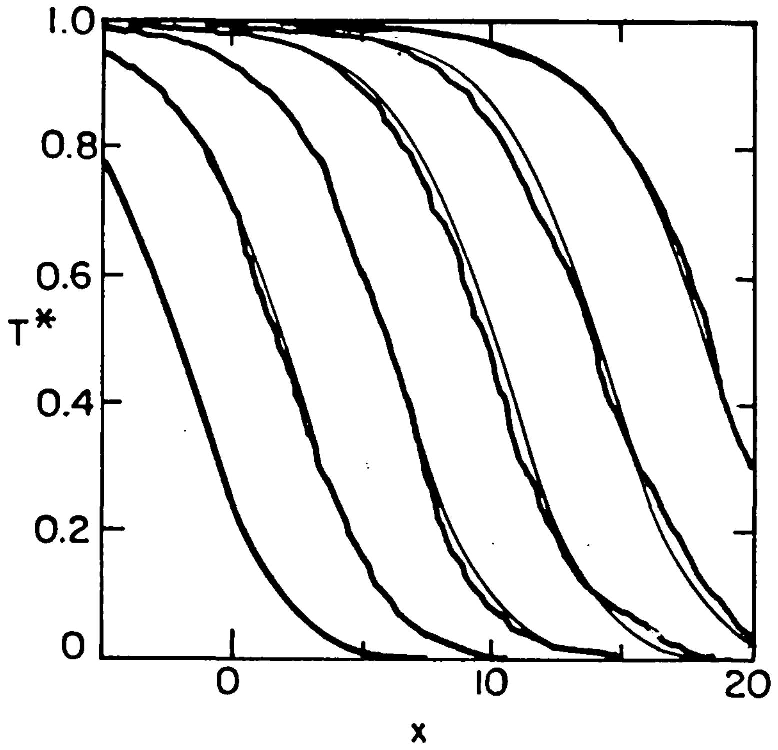
0
0
10
20
x

Fig. 8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0.6
T*
0.4
0.2
0
0
10
20
x

Fig. 9

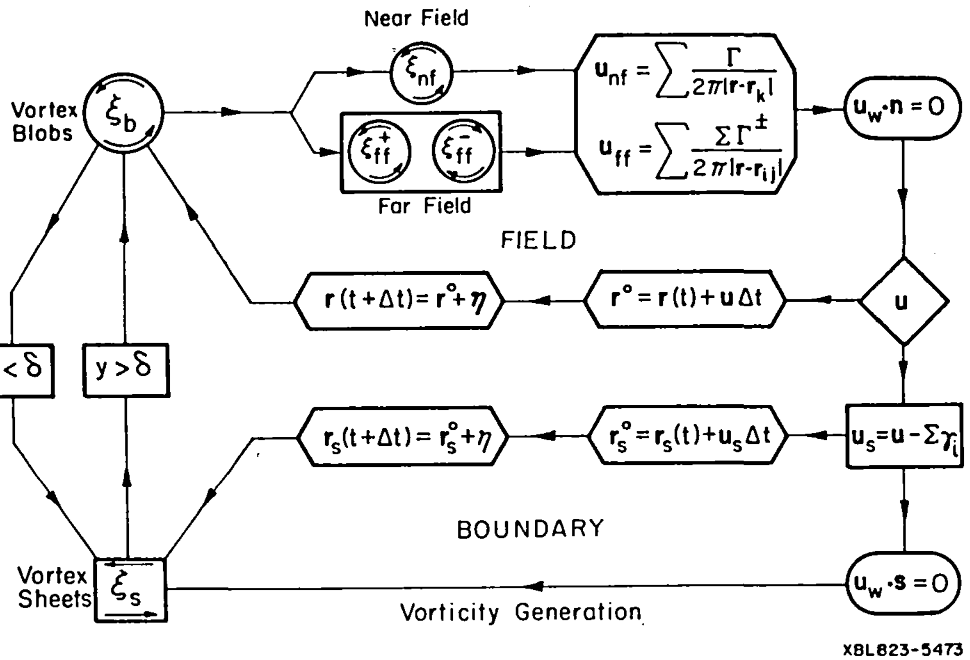
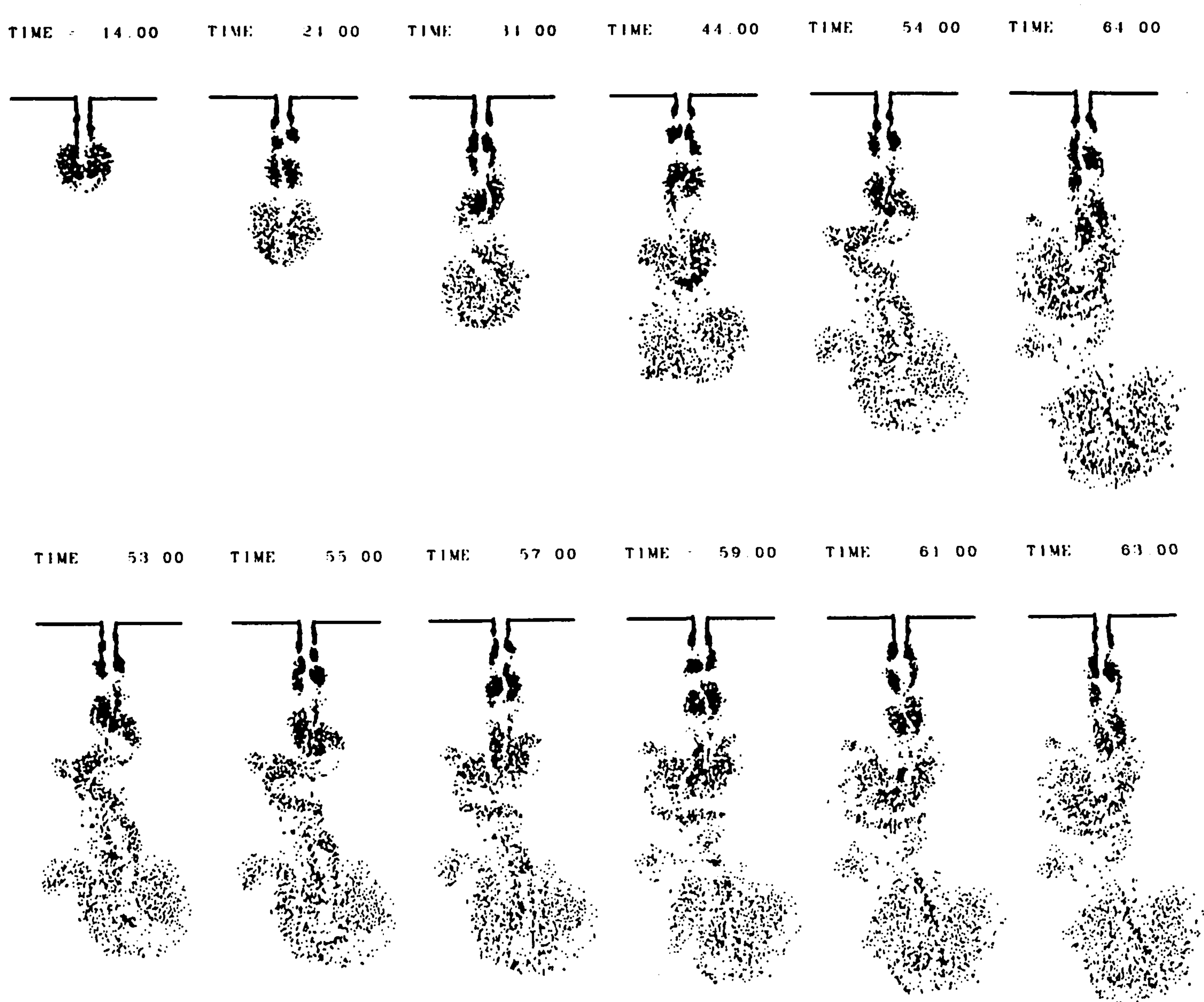

Near Field
Vortex Blobs
Far Field
FIELD
y < δ
y > δ
BOUNDARY
Vortex Sheets
Vorticity Generation
XBL823-5473

Fig. 10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TIME 21.00
TIME 31.00
TIME 44.00
TIME 54.00
TIME 64.00
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TIME 55.00
TIME 57.00
TIME 59.00
TIME 61.00
TIME 63.00

Fig. 11

COMBUSTOR FLAME FLASHBACK

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Objective: Analytically model and conduct basic experimental tests to study the fundamentals of flame flashbacks in combustors.

Background: Flashback has been a recurrent problem with the present Chrysler automotive gas turbine combustor. It can be a potential problem for other types and applications of advanced combustors as well. An improved understanding of the phenomenon would lead to improved design techniques to avoid its occurrence.

Approach: It is proposed to model, test, and develop the fundamental conditions and process by which flashback occurs on combustor wall surfaces. An atmospheric rig consisting of a small dump combustor with a premixing channel would be required. Operation would be on a gaseous fuel. The primary variables would be inlet air and wall temperatures (up to 1500° F), boundary layer thickness, gas stream velocities, and controlled pressure disturbance level in the combustor. Both steady-state and transient tests will be conducted.

Status: A steady-state flame flashback model is in existence. A transient model is being considered. The experimental rig is being designed. The experiment will be performed at NASA Lewis Research Center by a Case Western Reserve University student.

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