The Two-Fluid Model of Turbulence Applied to Combustion Phenomena

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Nomenclature

= body force component in x direction =interfluid friction constant = diffusion flux of fluid i= volumetric interfluid friction coefficient = volumetric fluid/wall friction coefficient = generalized flux of phase i= reciprocal of interface area per unit volume m_i = mass transfer rate into fluid i per unit volume p = pressure = volume fraction of fluid it =time и = velocity in x direction = velocity vector of fluid i= density of fluid i ρ_i = reactedness = general conserved fluid property = source of entity measured by ϕ

Subscripts

i = either fluid
 1 = fluid 1
 2 = fluid 2

Introduction

T has long been recognized that turbulent flames, like turbulent flows without combustion, are "spotty"; that is, that hot- and cold-gas fragments intermingle within a flame in the manner of an archipelago in the sea or a lake system on land. This concept was first expressed, so far as the present writer knows, by Shchelkin. Wohlenberg independently proposed something similar, with emphasis on the differences in the fuel: air ratio between the two interspersed gases. Howe and Shipman developed a mathematical theory for a uniform fuel: air ratio on the presumption that the interspersed gas fragments travel through the flame at equal velocities.

Recently, attention has been focused on the fact that the fragments may have significantly different velocities. Bray and Libby,⁴ who credit Kuznetzov⁵ with the first publication, explained how this arises from the different accelerations experienced by lighter and heavier gas fragments when subjected to the same pressure gradient. Their co-workers

Moss⁶ and Shepherd⁷ have provided experimental confirmation of this "slip" between the two phases. Phillips⁸ has recently published some calculations for flame propagation that incorporate this effect.

Making use of mathematical apparatus developed primarily for the analysis of two-phase flows, ¹¹ the author has proposed a general theory of turbulent flow, both with and without reaction, that is based on the two-fluid (i.e., "lakes and islands") idea. This theory allows the relative motion of the gas fragments to be computed, as well as their individual temperatures, fuel:air ratios, and states of completeness of reaction.

The "two-fluid" model of turbulence requires for its completion the determination of laws of fluid/fluid interaction in respect to heat, mass and momentum transfer, and fragment size changes. At present, these laws are only approximately known and comparisons with experimental data are needed for their better determination. Research of this kind is now in progress.

In the present paper, some results of this research are presented. Specifically, the mathematical theory is outlined and exemplary calculations are presented that emphasize the role of the pressure gradient on the rate of propagation of a transient one-dimensional turbulent combustion wave. Brief descriptions are also provided of how the model is being applied to other flame phenomena and of how it relates to earlier models proposed by the author.

The development of the model is still far from complete; however, the results presented here suggest that, when applied to turbulent combustion, the two-fluid model represents some important aspects of reality more faithfully than single-fluid models can.

Mathematical Formulation of the Two-Fluid Model

Definitions

It is supposed that two fluids, 1 and 2, share occupancy of space. The proportions of time during which each can be expected to occupy a particular location are called the volume fractions r_1 and r_2 . These obey, of course, the relation

$$r_1 + r_2 = 1 (1)$$

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How the two fluids are distinguished from one another is arbitrary; however, in combustion processes, the temperature and fuel:air ratio provide the most convenient distinguishing characteristics. In the calculations reprinted here, only premixed flames are considered; therefore, the two fluids are defined as "colder" (fluid 1) and "hotter" (fluid 2). However, the model is applicable to nonpremixed flames as well (see below).

At any location and time, all gas fragments belonging to fluid 1 are supposed to have the same values of temperature, mass fraction of component chemical species, velocity components, and fragment size. This assumption of fluid homogeneity is, of course, an idealization at variance with reality; but it may well lie closer to the truth than do the more conventional single-fluid models of flames.

All of the above fluid properties will be represented by the symbol ϕ_i , where *i* takes the value 1 or 2 according to the fluid.

It will be supposed that both fluids have the same pressure at each point—not because the equation system is significantly simplified thereby, but because no mechanism entailing a difference of pressure has yet been hypothesized.

Differential Equations

Mass Balances

There are two mass conservation laws to express. They can both be written in the form

$$\frac{\partial}{\partial t}(\rho_i r_i) + \operatorname{div}(\rho_i r_i V_i) = m_i \tag{2}$$

where t is the time, ρ_i the density of fluid i, V_i its velocity vector, and m_i the rate of transfer of mass into fluid i from the other fluid with which it is intermingled.

In Eq. (2), instantaneous values of ρ , r, V, and m are in question. Because it is impractical, in numerical calculations, to compute the most rapid fluctuations of these quantities, time-averaged quantities are preferable, in which case the quantity operated upon by div must be augmented by D_i , an effective diffusion flux. The equation then becomes

$$\frac{\partial}{\partial t}(\rho_i r_i) + \operatorname{div}(\rho_i r_i V_i + D_i) = m_i$$
 (3)

from which the overbars signifying time averaging have been omitted so as to avoid needless clutter. The $\partial/\partial t$ term is the difference of outflow from inflow along the time dimension, div that difference along the space dimensions, and m_i the negative of the difference between outflow and inflow along an "interfluid dimension." If all of these fluxes are denoted by G_i and DIV is defined as a generalization of div that makes reference to all their dimensions, Eq. (3) can be finally expressed as

$$DIV/(G_i) = 0 (4)$$

Balances of Other Quantities

The above nomenclature facilitates the compact writing of the differential equation governing the distribution of the fluid property ϕ_i . The equation becomes

$$DIV(\phi_i G_i) = \Phi_i \tag{5}$$

where Φ_i is the volumetric source of the entity ϕ in phase i and ϕ_i the value of ϕ associated with the flux it multiplies.

Of special importance are the momentum equations, in which ϕ_i is a velocity component. For these equations, the volumetric source quantity Φ_i consists primarily of pressure gradient, body force, and interfluid and wall friction terms.

Thus, for the velocity u_i , the equation becomes

$$DIV(u_iG_i) = -r_i\left(\frac{\partial p}{\partial x} + b_x \rho_i\right) + f_{ij}(u_j - u_i) - f_{iw}u_i$$
 (6)

where x is the distance coordinate aligned with u_i , p the pressure, b_x the body force component in the x direction, f_{ij} the volumetric interfluid friction coefficient, u_i the local velocity of the other component, and f_{iw} the volumetric coefficient of friction between fluid i and a nearby wall.

"Pressure Gradient" and Other Kinds of Diffusion

Because of the association of the fluid density r_i with each of the G_i on the left-hand side of Eq. (6) and of its nonassociation with the pressure gradient term on the right-hand side, the effect of the pressure gradient on the velocity components of the two fluids is inversely proportional to their densities. Therefore, pressure gradients cause the two fluids to have different velocities, so that they move relatively to one another.

Relative motion between intermingled fluids can also result from the random movements of fluid fragments, the net magnitude of which are usually proportional to the gradient of concentration (i.e., volume fraction). To distinguish the two phenomena, the present one will be here called "pressure gradient diffusion" and "ordinary" diffusion will correspondingly be called "concentration gradient diffusion."

Wider Significance of Pressure Gradient Diffusion

It may be interesting here to remark that, if the general theory of two-fluid turbulence is correct, pressure gradient diffusion can account for:

- 1) The enhancement of turbulent mixing as a consequence of curvature in a boundary layer on a concave wall.
- Its corresponding diminution in a boundary layer on a convex wall.
- 3) The interactions between gravity (and other body force) fields, gradients of density, and turbulence in the environment and elsewhere.
- 4) The special features of turbulence in strongly swirling flowfields.
- 5) The tendency of strongly accelerated flows to "laminarize."

Once its presence has been recognized at all, pressure gradient diffusion appears so prevalent that "ordinary" (i.e., concentration gradient) diffusion seems almost to be the exception rather than the rule. It is as though turbulence modelers have been too exclusively concerned hitherto with Kelvin-Helmholtz (i.e., shear-generated) instabilities and have consequently neglected the equally important Rayleigh-Taylor ones. At any rate, this is the viewpoint from which the present writer's current research is being planned.

Auxiliary Relations

Interfluid Friction

In order that the equation system should be "closed," i.e., rendered complete enough for solution, mathematical expressions must be devised for such interfluid transport quantities as m_i and f_{ij} . Since these questions have been discussed elsewhere, ^{9,10} it suffices here to indicate what formulas have been used in the computations presented below.

The formulation used for f_{ij} , which appears in Eq. (6), is

$$f_{ii} = c_f \ell^{-1} \rho^* |V_i - V_j| \tag{7}$$

where c_f is a dimensionless constant, ρ^* the density of the lighter of the two fluids, ℓ^{-1} the amount of fluid/fragment interface area per unit volume of space, and $|V_i - V_j|$ the local time-averaged relative speed of the two fluids.

The area/volume quantity ℓ^{-1} is taken as being proportional to the volume fraction product r_1r_2 , so that it vanishes when either fluid disappears.

In more advanced work,⁴ it is intended that a differential equation governing ℓ^{-1} be formulated and solved; in the present work, however, ℓ^{-1} has been taken as proportional to the reciprocal of the lateral dimension of the flow.

Interfluid Mass Transfer

The interfluid mass transfer process has been presumed to proceed in only one direction, namely, from colder (fluid 1) to hotter (fluid 2). This is not the only possible formulation and more symmetrical ones are being investigated by the present writer in other studies. However, it has some qualitative conformity with reality for combusting flows in which the change of state proceeds in only one direction.

The rate of mass transfer has been taken as directly proportional to the interfluid friction factor f_{ij} , the proportionality factor being in excess of unity.

Interfluid Heat Transfer and Diffusion of Chemical Species

Conductive heat transfer and diffusive transfer of chemical species between the two fluids have been neglected. Of course, the material passing from fluid 1 to fluid 2 carries its energy, momentum, and species contents with it; but the properties of fluid 1 are not affected by this transfer.

This presumption is justified in the same way as is the unsymmetric mass transfer assumption: All fluid elements affected by contact between a hot fragment and its colder surroundings are regarded as becoming part of fluid 2. By contrast, a transfer of momentum from fluid 2 to fluid 1 is allowed for by the finite value of f_{ij} . This difference from the transfer of energy and species is justified by the fact that the pressure effects can be exerted over greater distances than can those of heat conduction and viscous action.

Chemical Reaction Rate

The colder, unburned gas that is entrained by the hot fluid particles is *not* supposed to be burned instantly. Instead, reaction is taken to proceed by way of an idealized single-step Arrhenius reaction. Specifically, the rate of increase of "reactedness" τ is taken as proportional to $\tau^n(1-\tau)$, where n is an exponent of the order of five.

Reaction rate formulas of this kind have long been found convenient for the theoretical exploration of combustion phenomena (see, for example, Ref. 12). Only qualitative realism is claimed for them, but of a degree that is perfectly consistent with the objectives of the present study.

Solution Procedure

The solutions to be presented of the above system of equations have been obtained by straightforward application of a widely available and sufficiently documented computer program called PHOENICS. 11,13 Therefore, there is no need for further explanation here of the solution procedure except to note the main features embodied in PHOENICS:

- 1) The differential equations are replaced by fully conservative, fully implicit, finite-domain equations valid for a staggered and (in the present case) Cartesian grid.
- 2) Convection fluxes [i.e., all those represented by G_i in Eq. (4)] are computed from "upwind" values of r_i , ρ_i , and ϕ .
- 3) An iterative solution procedure is adopted that results in the diminution to below preset limits of all the imbalances in all the finite-domain equations.
- 4) A sufficient sample of the computations is repeated on successively finer grids (i.e., with smaller and smaller intervals of space and time) until the physically significant results are found to be independent of the interval size.

A full account of the computational details is provided in a PHOENICS demonstration report from the Imperial College Computational Fluid Dynamics Unit.²⁸

One-Dimensional Transient Confined Premixed Flames

The Process Simulated

Qualitative Description

In order to shed light on the role of "pressure diffusion" in turbulent combustion, a computer simulation has been made of flame propagation in a long duct. It is postulated that a two-fluid mixture is traveling uniformly along a constant-area duct, with both fluids proceeding at the *same* velocity. Therefore, at the start, there is neither friction nor mass transfer between the two fluids. The reactiveness of the colder gas is taken as zero and that of the hotter gas as unity.

It is further postulated that a shock wave travels through the mixture. This wave is caused by the sudden complete blockage of the duct at one end (how it is achieved is of no importance).

Of course, the shock wave is a concentrated pressure gradient. As it travels through the two-fluid mixture, it has a greater effect on the velocity of the hotter than on that of the colder fluid. Specifically, the former velocity changes sign, whereas the latter velocity does not.

What then ensues is easy to foresee: the finite relative velocity between the phases gives f_{ij} a finite value in accordance with Eq. (7). This leads to a finite rate of entrainment of fluid 1 into fluid 2. The reactiveness of the latter is lowered as a consequence of the mixing of cold fluid with hot; therefore, the chemical reaction rate becomes finite, in accordance with the law described above. The resulting decrease in the average density entails further changes in the pressure and velocity; thus, the pressure wave phenomenon is turned into a strong deflagration—or possibly even a detonation.

In the following section, some samples from the computation series will be presented. However, space limitations preclude description of all of the studies that have been made. The results are presented in graphic form with the aid of the line-printer-generated plots. Of course, full tabulations of numerical output can also be obtained if desired.

Relation to Other Phenomena

When considering the combustion wave implications of the calculations, some readers may want to keep in mind the similarity of the postulated mechanism to that believed to occur in "vapor explosions" of the kind that are much feared as potential complications during loss-of-coolant accidents in nuclear reactor systems. ¹⁴ There is no combustion in such explosions. The source of the energy is the temperature difference between coarsely distributed fragments of hot metal and the liquid coolant in which they are immersed. Unless an initiating pressure wave disturbs it, the process is a mild one: for vapor blankets, the metal fragments and limits the rate of heat transfer.

A pressure wave of sufficient magnitude can radically alter the situation for it sets up a relative velocity large enough to blow away the vapor blanket. Then, the heat-transfer rate is enormously increased, the pressure gradient and consequent velocity differences increase correspondingly, and the final result is a propagating wave of tremendous destructive power. One observed consequence is a fragmentation of the hot metal, that is, a finer-scale interspersion and an increase in the surface area per unit volume. It is simultaneously a result of increased relative velocity and a cause, through its effect in promoting heat transfer, of still greater relative velocity.

Quantitative Details

Just what values were chosen to define the computations is of very little importance; however, they should be stated in case others wish to verify the results. They were:

1) The pressure in the duct was 10^5 Pa initially and the densities of the hot and cold gases were 1.0 and 0.2 kg/m³, respectively.

- 2) Both gases were supposed to change density in proportion to $p^{1/1.4}$ and the hot-gas specific volume (i.e., $1/\rho_2$) was taken as linear in reactedness.
 - 3) The duct was 1 m long.
- 4) The initial gas velocity (for both fluids) was 10 m/s and the initial volume fraction of the hotter fluid was 0.1.
- 5) For simplicity, friction with and heat transfer to the walls of the duct were entirely ignored in the calculations presented.
- 6) For purposes of computation, the duct was divided into 50 equal intervals; 100 time intervals were employed, each of 10^{-5} s.
- 7) Tight tolerances were imposed on the residuals monitored during the computation. Therefore, it can be presumed that the solutions presented are fully converged.

Pressure Waves in the Absence of Mass Transfer Between Fluids

Cases Considered

In order to provide points of reference, the results of two calculations in which the mass transfer process was entirely suppressed will be presented first. In the first calculation, indeed, the second phase was absent; so all that occurs when the duct end is closed is that a pressure wave travels through the duct, bringing the fluid totally to rest.

Both phases are present in the second calculation, so the pressure wave acts differentially upon them in the manner described above. However, the resulting velocity differences are not allowed to give rise to the mass transfer, which alone can lead to further combustion in the present model.

Single-Fluid Wave

The results of the single-fluid computation are represented in Fig. 1 in the same form as will be adopted for all of the results. The plots represent the distributions of pressure and velocity along the duct 1 ms after the closing of the duct end. Along the top of the diagram are printed the maximum and minimum values between which each of the ordinates is plotted. It should be noted that pressures are measured as excesses above 10⁵ Pa.

Inspection of Fig. 1 shows that the pressure wave has an amplitude of 0.0387×10^5 Pa and brings the gas to rest. The speed of the wave, deduced from the distance from the closed end to the point where the pressure rise has 50% of its final value, is approximately 370 m/s, but another 5 m/s should be added to give its speed relative to the average of the undisturbed and the retarded gas masses.

These values can be compared with the theoretical speed of a small-amplitude pressure wave of $(\gamma p/\rho)^{\frac{1}{2}}$ i.e., $(1.4\times10^5/1.0)^{\frac{1}{2}}$ or 374 m/s, and with the corresponding pressure rise δu , $\sqrt{\gamma p\rho}$, i.e., $1060\times(1.4\times10^5)^{\frac{1}{2}}=3.74\times10^3$ Pa associated with causing the velocity change δu .

The agreement is as satisfactory as can be expected for results read from a line printer plot. Of course, the fact that the pressure rise is not as abrupt as in a real shock is a sign that numerical errors are still present; they would no doubt disappear if the grid size and time step were reduced.

Two-Fluid Wave

Figure 2 shows the distributions of pressure and velocity that prevail when the two fluids are present, initially in the volumetric ratio of 9:1. The time, 1 ms, is the same as before. Several differences can be observed:

- 1) The pressure rise is 0.0322×10^{-5} Pa, somewhat less than before; however, the wave has actually traveled 0.44 m, which is somewhat farther than it did in the single fluid.
- 2) It can be concluded that the colder-gas velocity has been reduced by the wave to the still positive value of 3.0 m/s; whereas the hotter-gas velocity has become negative, its value being -26.0 m/s.

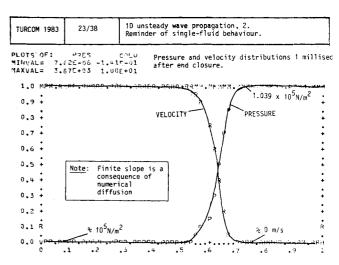


Fig. 1 Distribution of pressure (above atmospheric) and gas velocity in a duct in which the gas velocity is initially 10 m/s throughout. The left-hand end of the duct remains open, but the right-hand end is closed 1 ms prior to the occurrence of these distributions.

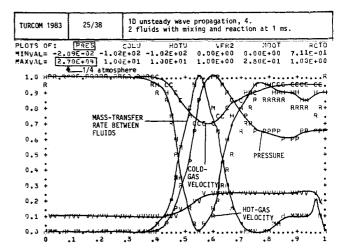


Fig. 2 Distribution of pressure and velocity in the duct 1 ms after the end is closed, when two gases are flowing, both initially at 10 m/s. The initial gas densities are 1 and 0.2 kg/m³; the lighter gas originally occupies one-tenth of the volume. Mass transfer between the two fluids is artificially suppressed. The pressure wave causes flow reversal in the lighter gas.

3) There are additional phenomena occurring near the right-hand end, where the slower colder gas tends to pile up, occupying a larger fraction of the volume than it did originally.

All these results are easy to understand. Their appearance is an indication that the computer code is in working order.

Two-Fluid Deflagration/Detonation Waves

Flame with Moderate Entrainment Rate Constant

Figure 3 represents the situation in the duct 1 ms after the passage of the wave when the ratio m/f_{ij} is taken as 20.0. The differences from Fig. 2, for which m/f_{ij} was zero, are very striking; they include:

- 1) The maximum pressure is now 0.27×10^5 Pa above atmospheric and the pressure distribution in the gas through which the wave has passed is nonuniform.
- 2) The velocity distributions are also highly nonuniform. The hotter gas is at one point traveling in the same direction as the wave with a velocity of 100 m/s.
- 3) The average speed of the wave, judged by the same criterion as before, is now nearly 500 m/s.

- 4) The volume fraction increases significantly as a consequence of the passage of the wave; but, even so, the proportion of unburned gas in the tube through which the flame has passed is still over 70%.
- 5) The interfluid mass transfer rate exhibits its peak just ahead of the pressure and, indeed, at the point at which the difference in the velocity between hot and cold fluids is a maximum.
- 6) This entrainment causes a reduction in the local gas reactiveness to just over 71%; however, it rises again after the wave has passed.

It is interesting to examine the earlier stages in the development of the wave, four of which are represented in Figs. 4-7. Inspection of this sequence shows that the wave is still in a state of development at the time of 1 ms. The peak pressures for the sequence of times have been 0.0415, 0.0669, 0.107, 0.170, and 0.270×10^5 Pa. A similar increase in wave strength is exhibited also by other variables.

Figure 8 represents the development in a different way; it shows values of pressure, velocities, volume fraction, etc. for a fixed location (viz, 25 cm from the closed end) throughout the first millisecond of the process. The pressure there has risen continuously, but the mass transfer rate has passed through a maximum and returned again to zero.

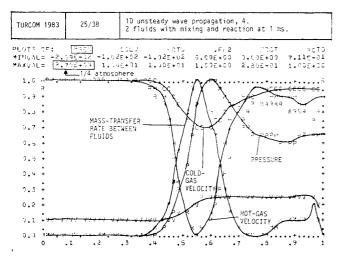


Fig. 3 Distribution of pressure, velocity, mass transfer rate, and other quantities 1 ms after closure of the right-hand end, after allowing for the mass transfer between the fluids and the subsequent chemical reaction in the hotter fluid. The pressure wave travels to the left with increased speed (compared to Figs. 1 and 2) and a pressure peak develops just to the right of the region of maximum mass transfer.

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Fig. 4 Flame of Fig. 3, 0.2 ms after closure of the right-hand end.

Effect of a Tenfold Increase in Entrainment Rate Constant

What happens when the entrainment rate constant is increased 10 times can be deduced from inspection of Fig. 4. Once again, the curves represent conditions in the duct at 1.0 ms after the start. Comparison can usefully be made with Fig. 3, which corresponds to the lower entrainment rate. This comparison reveals that the increased value of the constant has:

- 1) Raised the maximum excess pressure to 8.61×10^5 Pa.
- 2) Taken the wave almost to the open end of the duct.
- 3) Completely entrained the colder gas into the hotter (the volume fraction is close to unity).
- 4) Not yet caused it to react completely (the lowest reactiveness present in the hotter gas is 0.287).
- 5) Induced a maximum velocity of 581 m/s in the hotter gas in the direction of wave propagation.
- 6) Left the gas remaining in the duct still in a state of violent commotion.

It should be remarked that the high rate of entrainment is by no means physically implausible; it can result simply from the reduction in the size of the gas fragment. If lumps of metal can be reduced to powder by passage of a vapor explosion, there is certainly no reason to doubt that intermingled gas fragments can be just as rapidly comminuted.

In the calculations reported here, this further fragmentation effect has not been included. However, those in which it has been included (to be reported elsewhere) confirm that the influence on the process is a dramatic one.

Influence of Venting on the Flame Propagation Process

As has been emphasized, "pressure gradient diffusion" is the essential ingredient of the flame accelerations reported above. Therefore, it is to be expected that anything which can reduce the rise of pressure will also reduce the violence of the explosion. "Elastic" duct walls would have such an effect and so would the provision of "escape vents" through which the gases will tend to flow as their pressure rises.

Calculations illustrating the latter influences have been performed in the present investigation, some of which will now be reported.

The venting has been simulated by the provision of mass "sinks," linear in pressure excess, in both the continuity equations. The two cases presented here can be characterized as narrow and wide vent situations. The vents are supposed to run the full length of the duct. The calculations have been performed with the larger entrainment rate constant, which gave rise to the results shown in Fig. 9.

The narrow vent results are shown for comparison in Fig. 10. Comparison with Fig. 9 shows that the presence of the vent has the following effects: 1) the peak pressure excess is

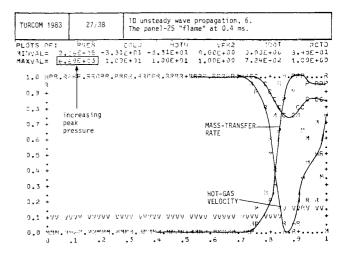


Fig. 5 Flame of Fig. 3, 0.4 ms after closure of the right-hand end.

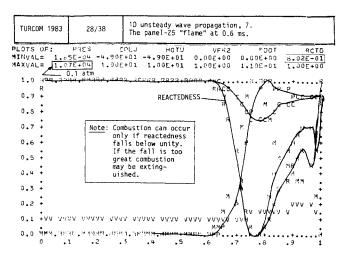


Fig. 6 Flame of Fig. 3, 0.6 ms after closure of the right-hand end.

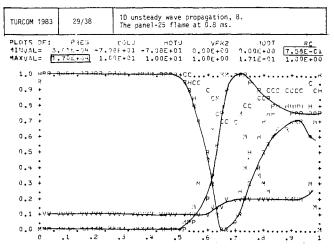


Fig. 7 Flame of Fig. 3, 0.8 ms after closure of the right-hand end.

only 1 atm, not nearly 9; 2) the wave has traveled only threequarters of the length of the duct; 3) the maximum negative velocity is only one-quarter of its previous value; and 4) the volume fraction of hotter gas, though still large, is not yet unity.

Figure 11 shows the corresponding results for the wider vent and reveals, as is easily understood, that the peak pressure is still lower, the wave travel distance is much smaller, neither fluid acquires a negative velocity, and the volume fraction of hotter fluid is everywhere quite modest.

It is clear that the two-fluid model does indeed display the tendencies that the experimental studies reveal. The provision of an escape route for gas diminishes the violence of the explosion; this is a consequence of hydrodynamic rather than chemical-kinetic aspects of the process.

Conclusions about One-Dimensional Transient Flame Studies

The present exploratory studies do no more than show that a realistic-seeming model has been created. There are many more influences to be explored and refinements of the physical inputs to the model are required.

Among the influences deserving exploration are those of 1) heat transfer to, and frictional effects of, the duct walls; 2) nonuniformities of fuel:air ratio of various kinds; 3) nonuniformities of duct cross section, including those which correspond to the presence of obstacles within the duct; and 4) the thermodynamic and chemical-kinetic properties of the gases in question.

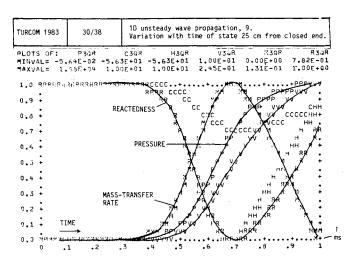


Fig. 8 Variations with time of pressure, reactiveness, mass transfer rate, volume fraction of the hotter fluid (V) velocities of the hotter (H) and colder (C) fluids at a location three-fourths of the distance along the pipe (i.e., 25 cm from the closed end).

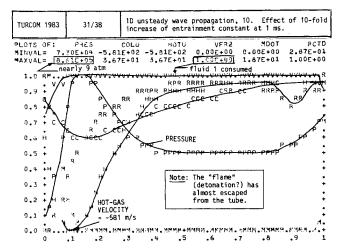


Fig. 9 Distributions of pressure P, fluid velocities H and C, reactiveness R of the hotter fluid, and other properties 1 ms after closure of the right-hand end and when the mass transfer constant is 10 times greater than for the flames shown previously.

Model features that could certainly benefit from refinement include: 1) the laws of interfluid mass transfer (i.e., entrainment); 2) the prescriptions of the fragment size or its deduction from a special differential equation; and 3) the possibility that, even though the net rate of mass transfer may be from colder to hotter, there is some significant transfer in the reverse direction that can be counted as interfluid molecular heat transfer and diffusion.

Study of these questions is not an expensive matter. None of the transient runs reported above required more than 15 min of CPU time on a Perkin-Elmer 3220 minicomputer; therefore, they would take less than 1 min on most mainframe computers. For many researchers, computer expenses of this order of magnitude are easily supportable.

Other Applications of the Two-Fluid Model of Turbulent Combustion

If it is to meet the needs of practicing engineers, the twofluid model of turbulence must permit prediction of both steady and unsteady phenomena in one, two, or three dimensions, whether reacting or not, all with the same set of auxiliary relationships and associated constants. Therefore, it behooves researchers on this subject to pay attention to more

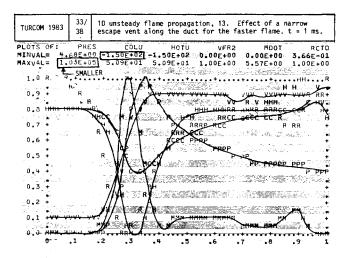


Fig. 10 Distributions of quantities of Fig. 9 under the same conditions, except that a narrow gas escape vent is provided along the whole length of the duct. The presence of the vent reduces both the maximum pressure and the propagation velocity.

than one type of turbulent flow in order that the "universality" of their recommendations should be subjected to test.

In the present writer's research team, some workers are concerned with nonreacting fluids, some with steady jets and boundary layers, and some with recirculating flows of various kinds. None of the research is yet far enough advanced for definitive results to have been achieved; but even the preliminary results are too voluminous to review comprehensively here. Nevertheless, a brief review of current and planned investigations may be of interest.

Two-Dimensional Steady Combustion Processes

A Ph.D. thesis¹⁵ is being completed that contains, together with the results of more conventional (i.e., single-fluid) modeling, two-fluid simulations of two types of (nominally) steady two-dimensional premixed flames confined in ducts.

The first type is that arising downstream of a centrally placed baffle in a plane-walled duct. Experimental data on flames of this kind have been presented by Williams et al., ¹⁶ Soln'tsev, ¹⁷ Wright and Zukoski, ¹⁸ Howe and Shipman, ³ and many other authors. Several attempts at the creation of a suitable mathematical model of the process have been made by the present author in earlier publications. ¹⁹⁻²²

The second type is that occurring downstream of a "step," i.e., of an abrupt enlargement of width, in a duct supplied with a steady combustible stream. Experiments of this kind have been reported by Ganji and Sawyer,²³ Pitz and Daily,²⁴ and probably others.

Flames of the first kind are "parabolic" in character; a "marching integration" in the flow direction suffices for the solution of the equations. Those of the second kind are "elliptic," which implies that an iterative solution of the equations must be obtained, valid for the whole two-dimensional domain simultaneously.

The same computer program (PHOENICS) is employed in this work as was used for the computations reported above. The modeling assumptions are the same, except that:

- 1) The interphase friction coefficient is not allowed to fall to zero with the relative speed of the two fluids, but retains a lower-limit value representative of the random turbulent motion (for which various assumptions are under exploration).
- 2) Turbulent transport of the fluids (i.e., intermingling as a consequence of random motion across time mean streamlines) occurs at a rate proportional to the product of the gradients of volume fraction and velocity.
- 3) This turbulent transport, because the diffusing fluid fragments carry the momentum prevailing at their points of origin, has a consequential effect akin to that of viscosity.

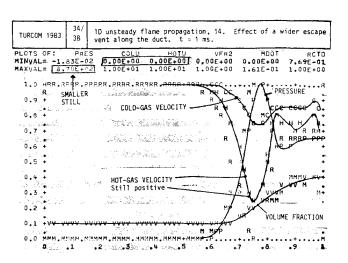


Fig. 11 Distributions of quantities of Fig. 9 under the same conditions when a wider vent is provided along the length of the duct. The flame phenomenon is now very much milder.

Because of the number of choices to be made as the model is constructed—choices that may be inspired by intuition, but must be checked meticulously against experiment in respect of *all* their qualitative and quantitative implications—development of the model proceeds at a slower pace. Nevertheless, it is already possible to conclude that the experimental data *can* be fitted satisfactorily and, indeed, that predictions can be made of quantities which previously evaded analysis.

For example, "intermittency" is a dominant feature of the Pitz-Daily flame; this appears in the present model as a volume fraction of the hotter fluid (which is well below unity) coupled with a large gas fragment size. Ability to accommodate such observations within its theoretical framework is, the present author believes, one of the most attractive features of the two-fluid model.

Two-Dimensional Transient Confined Flames

Flames stabilized by baffles in ducts may be present in the exhaust ducts of aircraft jet engines that require extra thrust for short periods. The baffle/duct arrangement is then called an "afterburner" or "reheat" system.

Although the flow in such systems is intended to be steady, experience has shown that oscillations may easily occur, their amplitudes often being of such a magnitude as to cause damage. The mechanism appears, from experimental studies by Campbell et al.²⁵ to be this: 1) a pressure wave travels upstream along the duct; 2) its influence on the hotter and colder streams is of the kind shown above, i.e., such as to increase the local burning rate; 3) a rarefaction follows having the opposite effect; 4) the resulting unevenly burned gas stream passes downstream to the exhaust nozzle, where its unevennesses of mean density interact with its flow vs pressure difference characteristic in such a way as to create a succession of compression and rarefaction waves which travel upstream. The process thus sustains itself.

This process is also under investigation by the author's research team, the computer program and two-fluid model being identical with those described above. Of course, the transient form of the equations must again be employed and suitable boundary conditions are needed for the representation of the exhaust nozzle and upstream supply characteristics. This research is still in its early stages.

Steady Two-Dimensional Unconfined Nonpremixed Flames

One of the turbulent flames to which much experimental and theoretical research attention has been devoted is that resulting from the upward injection of a fuel gas into a surrounding atmosphere of nonmoving air. Despite the extensive research, it remains true that no existing mathematical model simulates all of the observed features of these flames very well.

Flames of this type, usually called "turbulent diffusion flames," are now being simulated by the author's research team by means of the two-fluid model. The model and computer program are the same as those already described, except that an additional equation must be solved, namely, the "mixture fraction" (i.e., for the proportions of the mass present in either of the fluids that originated in the injected fuel).

Transient Two-Dimensional Unconfined Nonpremixed Flames

There is much practical concern and research interest in "vapor-cloud explosions" in the atmosphere, i.e., those combustion phenomena that arise when a body of combustible gas released into the atmosphere first mixes, at least partially, and then burns because of contact with an ignition source. This phenomenon is also under study by the present writer's research team, the theoretical ideas being essentially those already described—just the initial and boundary conditions are different.

The gravitational terms in the momentum equations are especially important in phenomena of this kind. When the released fuel gas is denser than the atmosphere, it often spreads over the ground like a spilled liquid and mixing at the top of the layer may be inhibited by what can truly be called "countergradient diffusion." The pressure diffusion forces lighter fluid (air) upward toward a region where the concentration of lighter fluid is already high, thus separating from the denser fuel gas.

What happens when the ignition source takes effect is extremely dependent upon the timing and location of that source and upon whether partially confining walls or embedded obstacles allow the development of pressure gradients that can promote mixing and combustion in the manner described above. The research is directed first toward understanding the various scenarios qualitatively and then simulating them quantitatively.

Experiments are being conducted in the first instance with liquids of differing densities so that the initial nonreacting phase of the process can be simulated in the laboratory as well as in the computer.

Two-Fluid Model in Perspective

As mentioned above, the author has made earlier attempts to create satisfactory models of turbulent flows; thus, an explanation of how the present model relates to the previous ones is appropriate.

A 1959 paper 19 presented the idea of hotter and colder streams acted upon differentially by the same pressure gradient and thus caused to have differing velocities. The assumption was made that the entrainment across the stream boundary of the cold gas by the hot one, at a rate proportional to the velocity difference, limited the rate of combustion. At that time, the hot and cold streams were regarded as flowing side by side, whereas in the present model they are allowed to intermingle; but the two models have concepts in common.

The same thinking underlay another paper²⁰ in 1967; but a computer was then employed to integrate the equations.

By 1970, attention was being focused upon the *continuous distribution* of gas properties within the flame, which was no longer artificially divided into burned and unburned streams. This required devising formulas for the volumetric reaction rate, one of which was the "eddy-breakup" model in which the time-averaged velocity gradient was regarded as the main determinant of the rate. This notion also bears a resemblance to the two-fluid model, in which the place of velocity gradient is taken by the velocity difference between the fluids, divided by the fluid fragment size. A paper²² in 1973 sought to replace the velocity gradient by the ratio of the turbulence energy-to-dissipation rate; this was later perceived not to be an advance.

In none of these models did it seem possible to find a place for chemical-kinetic influences to be exerted; yet it was known that even highly turbulent flames did exhibit chemical-kinetic effects. The author's solution to the problem was his so-called "ESCIMO" model, discussed in a series of papers²⁹⁻³³ published between 1976 and 1982. The last of these papers, in which the model was compared with experimental data on hydrogen/air "diffusion" flames, concluded that the ESCIMO model was representing only what was (perhaps) occurring in the hot fragments of gas. It drew attention to the need for a theory that calculated how the space was shared between them and the cooler gas fragments with which they intermingle. The two-fluid theory is the answer to that need; and, until it has been sufficiently developed, it has seemed to the author that further ESCIMO model development is not needed.

The two-fluid model does therefore appear to be a logical experience-guided extension of earlier ideas. What is regrettable, however, and hard in retrospect to understand, is how long drawn out the progress has been.

Conclusions

The "spottiness" of turbulent flows generally, and of combusting ones in particular, is not likely to be disputed by those who are acquainted with experimental observations; so the ability of the two-fluid model to account for it quantitatively can reasonably be regarded as giving that model better-than-usual prospects of success.

For these prospects to turn into realities depends upon whether:

- 1) Single-fluid models can, after all, be developed so as to take better account of intermittency and related features of real turbulence.
- 2) The still-open questions related to the two-fluid approach are answered judiciously and with reasonable dispatch.
- 3) The "spottiness" will prove, when further studied, to be so extreme as to demand a multifluid model for its representation and, moreover, one that is so complex and expensive to operate that it cannot be used in practice.

The determination of these questions must be left to the future.

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