REACTING FLOWS AND COMBUSTION

Stephen B. Pope
Mechanical and Aerospace Engineering Department
Cornell University
Upson Hall
Ithaca, NY 14853-7501

INTRODUCTION

The practical importance of combustion is matched by its difficulty as a scientific discipline. The next three paragraphs illustrate the importance of combustion in energy conversion, fires and explosions.

Oil or coal-fired power plants, aircraft and automobile engines all depend on the combustion of fossil fuels. Vast amounts of fuel are consumed annually, with commensurate emissions of atmospheric pollutants. A major goal of combustion science and engineering is to understand the fundamental combustion processes better, so that the performance of these energy-conversion devices can be improved, leading to reduced fuel consumption and pollutant emissions.

Fires are responsible for upwards of five thousand fatalities and tens of billions of dollars in losses annually in the United States alone. They also represent a significant environmental hazard, particularly in connection with industrial accidents such as those associated with the extraction, transport and processing of petroleum products. Finally, the oil field fires in Kuwait demonstrate that fires on an enormous scale can pose public health and climate impact problems on a regional and perhaps global scale.

The study of detonative combustion goes back to the l9th century, driven by the desire to understand and thereby prevent coal mine explosions. Explosions still plague, not only mining operations, but also arise in grain elevators, fuel handling facilities and many other industrial operations and are particularly destructive when they involve detonations. There is also recent concern regarding detonative explosions within space vehicles or during the launch of liquid hydrogen-oxygen rockets, and in the case of the Three Mile Island accident there was the possibility that the hydrogen generated during core meltdown might detonate and cause rupture of the reactor containment.

Combustion is an extremely difficult phenomenon to study for several different reasons. While the gas phase is usually dominant both solid and liquid phases can be present for example in the form of coal particles, oil

droplets, and soot. Even in the gas phase, the chemistry is complex: typically there are about 50 chemically-significant species participating in perhaps 200 significant reactions. These coupled reactions have time scales varying from $10^{-12}s$ to $10^{2}s$.

The coupling of the thermochemistry with the fluid mechanics can be strong, and leads to further complications. The high temperatures involved (e.g. 2,000 K) lead to property variations (e.g. density and viscosity) of a factor of ten or more. The short reaction time scales in conjunction with the fluid mechanics leads to short length scales, for example flame thicknesses of a tenth of a millimeter. In most practical applications the flows are turbulent, leading to the phenomenon of turbulent combustion–the intersection of two non-linear problems with multiple scales. The short length and time scales involved, together with the high temperatures present a significant challenge to experimental investigations.

In spite of these considerable difficulties, in the last ten years great strides have been made in understanding combustion, both experimentally (largely through the development of laser diagnostics) and theoretically (largely by the exploitation of more powerful computers).

It appears that the available tools are now a match for the complexities of combustion, and that significant progress can be expected in the next decade.

RESEARCH

Combustion is a broad discipline, with a wide variety of applications. The present exposition cannot be comprehensive. The following sub-sections illustrate just some of the currently-active research areas.

Laminar Flame Studies

Emphasis on improving the efficiency of power generating units combined with the modeling of turbulent reacting flows and environmental issues dealing with the production of nitrogen based pollutants helps to motivate the study of laminar flames. As an example, most of the oxides of nitrogen are formed during combustion when part of the oxygen combines with atmospheric nitrogen rather than with the fuel. As a result, the burning of hydrocarbon fuels can produce large quantities of NO and NO_2 (nitric oxide and nitrogen dioxide, respectively). Both compounds are considered toxic and nitrogen oxide is related to the formation of photochemical smog. Laminar flames can help elucidate the processes by which NOx is produced in combustion systems.

In the late 1970's and early 1980's, there were definitive computational studies of one-dimensional laminar flames. The conservation equations were

solved numerically with detailed combustion chemistry and transport properties, and the results were shown to be in accord with experimental observations.

The study of the interaction of heat and mass transfer and chemical reaction in practical combustion systems requires a multidimensional study. Three-dimensional models combining both fluid dynamical effects with finite rate chemistry are as yet computationally infeasible. As a result, the modeling of chemically reacting flows has generally proceeded along two independent paths. In one case chemistry was given priority over fluid mechanical effects and these models were used to assess the important elementary reaction paths in, for example, hydrocarbon fuels. In the other case, multidimensional fluid dynamical effects were emphasized with chemistry receiving little priority. It is only within the last couple of years that the modeling of laminar flames has begun to consider the complex interaction between the fluid dynamic and thermochemistry solution fields.

The relatively recent movement into multidimensional systems is due in large part to the size of the systems that must be solved. In computational fluid dynamics (CFD) computations one often solves the Navier-Stokes and continuity equations for the velocities and pressure as a function of the independent spatial coordinates. In computational combustion the fluid dynamic equations are coupled to the energy and species balance equations. While CFD computations rarely solve for more than five unknowns, this is not the case in reacting flow computations. In particular, for laminar hydrocarbon flames one often solves for as many as 30 chemical species in addition to the temperature and the fluid dynamic variables.

In addition to the accurate prediction of the basic combustion process in multidimensional systems, the concept of fluid dynamical control of the combustion process is an extremely important issue for a variety of combustion systems. As an example, the lean extinction limit of premixed methane-air flames as measured in the laboratory at atmospheric pressure occurs at a stoichiometric ratio of about 0.5. However, when counterflowing streams of premixed methane and air are counter rotated, a compression zone develops near the stagnation point. This effectively reduces the straining on the system and the flame is able to sustain combustion at lower equivalence ratios than if no rotation were present. In particular a 10-15% reduction in the lean extinction limit can be obtainable in a two-dimensional counterflow configuration. Application of this concept to practical burner systems has not yet been undertaken but the potential is clearly significant from the point of view of lowering CO and NOx levels for gas turbines and home furnaces and in decreasing the thermal stress on system components.

Fluid dynamic considerations are clearly of importance in the modeling of the laminar combustion system. The ability to predict accurate fluid and

chemical fields in multidimensional flames will inevitably lead to a better understanding of the processes by which pollutants are formed, in improving engine efficiency and in modeling turbulent reacting flows.

Optical Diagnostics

In a combustion environment, the measurement of fluid velocity, temperature or chemical species concentration is complicated by changes in density, due to heat release, concomitant with mixing of two or more streams. The high temperatures melt delicate probes; probes that do not melt are too large to resolve the fluctuations in the flow. Nonintrusive optical diagnostics are called for. Laser Raman scattering from a single microsecond laser pulse, has produced time resolved measurements of scalars in turbulent flows. These new measurements are most successful when the experiment and the diagnostic are designed in concert. In turbulent nonpremixed flames, high mixing rates lead to flame extinction. It is easy to see the effects of local flame extinction with pulsed Raman scattering. Thus, the laser here is a binary diagnostic that tells us when the mixing rates have exceeded a critical value. By systematically changing fuel and the mixing geometry, the binary signal from the laser Raman becomes a powerful tool for interpretation of turbulent mixing rates. Flame extinction is an abrupt process whose nonlinearities will challenge models in the extreme. As an intermediate challenge, we have explored mixing rates and chemical kinetic rates, without flame extinction. Fuels that contain an oxidizer have been used to explore the competition between mixing (dilution in coflowing air, typically) and reaction. At high mixing rates, the oxidizer in the fuel has little time to convert fuel on the 'rich side' to products, so the oxidizer is a passive scalar. At lower mixing rates, the oxidizer in the fuel has time enough to attack the fuel and so a change is observed using the laser Raman scattering probe. This combination of laser diagnostic and judicious choice of fuel and geometry will continue to be a fruitful avenue of research.

A common assumption in models of turbulent combustion is that all species, and heat mix and diffuse at the same rate. This assumption produces great simplification in the modeling; yet we should have some notion of effects of differential diffusion. Only recently have we been able to isolate the different effects. Laser probing of nonreacting mixing of a jet of propane and hydrogen mixing with air have shown local separations of hydrogen from propane. These point laser measurements quantify differential diffusion but also lead us to consider the nature of large scale mixing as it effects the molecular level.

In the immediate future we can expect further evolution from single point measurements to two dimensional planar images of laser Raman and planar laser induced fluorescence, PLIF. PLIF images will improve our qualitative

view of turbulent mixing. It is reasonable to expect a PLIF sequence of images. For combustion flows, the rapid time scales lead us to imagine that the images will be acquired through a combination of multiple cameras and lasers. For nonreacting turbulent flows, such images are already appearing. In addition, the slower time scales associated with laboratory liquid mixing flows allow the planar images to be scanned in space, yielding a three dimensional image of a mixing flow. By collecting many of these three dimensional sets in sequence, a full three dimensional plus time measure is now emerging. These measurements are the experimental analog of direct numerical simulation. As before, much will be learned from these liquid injection experiments that will be extrapolated to gas phase flows and extrapolated further to combustion flows.

Much interest in combustion is due to the formation of pollutants and toxics at a heretofore acceptably small level. These small concentrations are weakly linked to the major reactions in combustion. The numerical prediction of such pollutants, such as nitric oxide and carbon monoxide, is a challenging, but urgent, area of research. Analogously, the measurement of part-per-million species in the surrounding environment provided by turbulent combustion is a challenging, but urgent, area of research. An emerging diagnostic has the intimidating name of Degenerate Four Wave Mixing (DFWM). Suffice to say, research on laboratory laminar flows is showing great sensitivity to part-per-million species with the challenges of a signal that is nonlinear with respect to laser power and species concentration.

Computer Modelling of Turbulent Combustion

In recent years, turbulent combustion models have seen increased use in the design and development of combustion devices including: gas-turbine combustors, furnaces, boilers and internal combustion engines. The aim of these models is to determine the performance of a proposed design, where "performance" may include heat-transfer and temperature-field characteristics, pollutant emissions, and interactions with mechanical components.

Models currently employed are found to be useful even though they are limited both in accuracy and in scope. Typically they are finite-volume codes in which the Reynolds-averaged conservation equations are solved in conjunction with the $k-\epsilon$ turbulence model. Combustion may be assumed to be mixing-limited, in which case finite-rate kinetic effects are not represented.

To meet all practical design needs, current turbulent combustion models need to be improved in the following respects:

i. generality,

ii. finite-rate kinetics,

iii. accuracy of turbulence modelling,

iv. incorporation of additional effects.

Most models are applicable either to diffusion flames (with a single fuel stream and a single air stream) or to premixed flames (in which the reactants are thermochemically uniform). Many important combustion processes are not well approximated by these idealizations. Examples are: staged combustion, piloted diffusion flames, stratified charge engines, and inhomogeneously premixed flames (as may occur in two-stroke engines).

The major improvement currently being sought is the ability to handle realistic finite-rate chemical kinetics. There are two motivations. The first is to calculate the effects of "slow" reactions, such as the production of NO_x and soot, or the post-flame oxidation of CO. The second and much more difficult objective is to calculate ignition, extinction and related phenomena.

There is considerable current research to develop more advanced models that can meet these needs. One approach is PDF methods in which a modelled transport equation is solved for the (one-point, one-time) joint probability density function (pdf) of the fluid properties. A major attraction of this method is that the direct effects of reaction appear exactly in the pdf equation, and hence require no modelling assumptions.

More comprehensive models (such as the pdf method) inevitably result in a computational problem that is one or more orders of magnitude greater than that generated by currently used turbulent combustion models. However, with the rapid advances in computer hardware (especially parallel processing), it is likely that hardware will not be a limiting factor. Algorithm development will be needed, however, to combine more comprehensive models with parallel machines to produce a useful design tool.

The above discussion pertains to turbulent combustion models with a direct engineering objective. Another valuable approach with a different objective is Direct Numerical Simulation (DNS). Here the idea is to solve the conservation equations without modelling assumptions, with the scientific objective of gaining a better understanding of the basic physical and chemical processes involved. Compared to DNS of non-reactive flows, this is a very difficult task–arguably one that is infeasible with current computers.

In practice, to yield a tractable computation, severe modelling assumptions are made–not for the turbulence, but for the thermochemistry. For example, a one-step reaction and equal species diffusivities may be assumed.

Spray Combustion

Sprays and spray combustion are complex and challenging because they involve numerous unresolved problems from a variety of scientific disciplines;

for example, liquid breakup through interface instability, dispersed multiphase flow, turbulent mixing, thermal radiation in participating media, interphase transport in a reactive environment and the chemical kinetics of flames, among others. Thus, although scientific study of spray combustion began with single drop combustion studies nearly fifty years ago, current understanding of spray combustion is still very limited. This is unfortunate because sprays and spray combustion are critical technologies for energy conversion and pollutant production–major concerns that will become even more important in the future as fuel supplies dwindle and sources of pollution multiply.

Research accomplishments and needs for combusting sprays are discussed in the following, emphasizing fluid mechanics issues. The discussion begins with single drop processes and concludes with sprays.

The vaporization and combustion of single drops have received considerable attention because they are well-defined and important unit processes for sprays. Thus, the general mechanisms of drop vaporization, ignition, combustion and extinction are understood and there is empirical information available to estimate drop transport rates for engineering purposes at moderate pressures. Nevertheless, understanding of drop transport properties for conditions relevant to practical combusting sprays is far from complete. The main difficulties are that drops are fluid rather than solid particles, and that drop transport occurs in a turbulent environment.

Current knowledge about drop transport is based on concepts derived from solid spherical particles. In actual practice, however, drops deform, have internal motions and are subject to secondary breakup. These real processes are particularly important for practical combustion devices. For example, at the high pressures of many practical combusting sprays, drop surfaces approach the thermodynamic critical point where reduced surface tension causes effects of deformation and internal motion that have received little attention. Additionally, recent studies show that drops formed by primary breakup at liquid surfaces are intrinsically unstable to secondary breakup, yet the dynamics and outcome of this rate controlling process are unknown.

Drops in combusting sprays are in a turbulent environment where they experience high relative turbulent intensities and scalar property fluctuations (e.g., velocity fluctuations comparable to the mean relative velocity between the phases and temperature fluctuations on the order of 500 K). This causes two effects that are significant for transport in sprays: turbulent dispersion of drops, which is an important turbulent mixing mechanism, and enhancement of drop transport rates by temporally and spatially varying surroundings. Problems of turbulent dispersion of drops are receiving increasing attention, which should be encouraged due to the importance of this multiphase mixing mechanism. Drop transport rates in turbulent environments have received

some attention in the past, but better understanding of this process should result from application of modern experimental and computational diagnostics.

Sprays are frequently divided into two categories: dense sprays, which involve the high liquid volume fraction region near the injector where processes of liquid breakup and the presence of irregular liquid elements (e.g., ligaments) are dominant features; and dilute sprays, which involve the low liquid volume fraction region more remote from the injector where drops are more or less spherical and processes of drop transport and turbulent dispersion are dominant features. Thus far, there have been relatively few studies of combusting sprays for either regime because the complexity of these flows already make nonevaporating and noncombusting sprays difficult to measure or analyze. One can sympathize with the desire to reduce complexity by avoiding combustion: however, measurements of the structure of combusting sprays are feasible using contemporary instrumentation and experiments along these lines are needed to highlight unit processes that merit additional study and to gain a better fundamental understanding of combusting sprays.

The main uncertainties about sprays are associated with the dense spray region. This region is crucial because it controls the properties of drops entering the dilute spray portion of the flow. In spite of its importance, however, dense sprays have not been studied very much due to problems of penetrating dense drop clouds with experimental diagnostics. Lack of experimental observations has correspondingly impeded the development of theory. Recent developments, however, have changed this picture appreciably and there is now significant potential for observations of dense sprays that should yield a period of rapid growth in understanding this flow. The main new tools have been the development of holography techniques capable of penetrating dense sprays and even observing processes of primary breakup along the liquid surface, as well as exiplex techniques for resolving liquid and vapor concentrations. Results thus far have shown that existing theories of primary breakup based on stability theory are ineffective and have disclosed a new turbulent breakup mechanism that is active in some instances; therefore, much remains to be done to gain a reasonable understanding of this first step in any spray process. Additionally, secondary breakup processes in dense sprays appear to involve mechanisms of ligament stretching and turbulent distortion that have not been considered in classical shock tube studies of the breakup of round drops.

Another facet of sprays, relevant to both dilute and dense sprays, is the effect of turbulence/dispersed-phase interactions on the turbulence properties of the continuous phase. Two interactions are important in principle: turbulence generation by the stirring action of drops moving with a velocity relative to the continuous phase; and turbulence modulation (damping) by

interactions between the velocity fluctuations of the drops and the continuous phase. Turbulence modulation has received greatest attention in the literature, however, this effect is more significant for sedimentation than sprays. On the other hand, turbulence generation by drops creates the turbulence field of dense sprays and this type of turbulence has distinctly different properties from conventional single-phase turbulence. These differences will no doubt attract study of turbulence generation by drops (particles) in the future, which might provide a useful perspective for a better understanding of conventional turbulence as a by-product.

The other side of turbulence/dispersed-phase interactions is turbulent dispersion of drops which was mentioned earlier in connection with studies of individual drops. However, recognition that turbulence within dense sprays differs from conventional turbulence implies a need to study turbulent dispersion in spray environments as well. Recent work has disclosed features of turbulent dispersion that merit particular attention: self-generated dispersion where eddy shedding from drops causes them to disperse laterally even in quiescent gases, and effects of unsteady turbulent flow fields on drop dynamics and transport due to effects analogous to virtual mass, Magnus, Basset, Saffman lift, etc., forces but for Reynolds numbers higher than the Stokes regime that are more representative of drops in sprays.

To summarize: issues for single drops include effects of deformation and motion of drop liquid on interphase transport, and the effects of a strongly turbulent environment on transport to droplets and turbulent dispersion of drops. Issues for sprays include the mechanism of primary breakup for non-turbulent and turbulent liquids, the relevant secondary breakup mechanisms for dense sprays, turbulence generation by drops in dense sprays, and the dynamics of interactions between drops and turbulence representative of practical spray combustion processes. Progress toward gaining an understanding of these problems has been slow in the past, however, recent development of instrumentation capable of resolving processes within sprays, and continued growth of computational capabilities, offer exciting prospects for rapid advances in the future.

Fire Research

The fluid mechanics of fires is of interest for two distinct reasons. First, the combustion processes in most fires are controlled by the turbulent mixing of the gas field fuel and air into a buoyant plume. A portion of the chemical energy released is then fed back to the condensed fuel surfaces by a combination of convective and radiative transport to sustain the fire. Second, the buoyant plume generated by the fire acts as a giant pump, distributing heat and hazardous combustion products over a much broader domain outside the active combustion zone. The transport and dispersion of smoke and

hot gases is controlled by the interaction of buoyancy driven flows with the geometric and ventilation constraints imposed by building environments or the meteorological and topographical conditions in the vicinity of outdoor fires.

The above division of interests is reflected in the advances made over the past decade. Most of the progress in fire related combustion processes concerns the structure of free standing fire plumes with known burning rates. The time-averaged velocity, temperature and plume width in purely buoyant plumes inside and outside the combustion zone has been measured as a function of position and correlated with the global heat release rate over a four order of magnitude range of fire strengths. The utility of the mixture fraction (the fraction of material at a given point in the flow that is or was fuel) as a correlator of temperature and major species in both buoyant jets and plumes has been demonstrated for a variety of simple fuels. Finally, the existence of large scale structures in the form of reasonably periodic toroidal pulsations of the entire plume has been demonstrated and plausible correlations of frequency with fire size developed. Indeed, the state of knowledge with respect to fire plumes at present is quite analogous to that of turbulent mixing layers shortly after the famous Brown-Roshko experiments in the early 1970's.

The understanding of plume structure together with other advances in fire driven flow have led to the development of fairly comprehensive mathematical models of smoke and toxic gas transport in complex building structures. These are lumped parameter models with an individual room divided into a hot upper layer, a cold lower layer, and fire plumes where required by the scenario under consideration. Separate studies of flows through doorways, convective and radiative heat transfer to boundaries and catalogs of burning rates of common furnishings have helped these "zone models", as they are known in the fire research community, to become practical engineering tools. More recently, commercially available computational fluid dynamics codes have been adapted to study fire induced flows in enclosures of complex shape, and large eddy simulations based on approximations to the basic fluid dynamics equations in simple geometries have also been performed. The "nuclear winter" scenario has led to a revival of interest in the properties of large fires. The first models intended to explicitly account for some of the fluid mechanical issues raised by such fires, together with the beginnings of a relevant field scale experimental data base, have begun to appear.

The level of sophistication of most of the fluid mechanics related to fire research is still primitive compared with that in other branches of fluid mechanics. The fire plume is as central a fluid mechanical entity to this subject as the mixing layer is in other branches of fluid mechanics and deserves a comparable level of effort. Studies of burning surfaces are either focused on the solid phase phenomena or conducted at a scale sufficiently small for

stable laminar flow to exist. More realistic investigations of the coupling between gas and condensed phase phenomena are in their infancy. The application of "zone" models to very large buildings awaits the development of usable, experimentally validated theories of smoke movement down long corridors and in vertical shafts. The role of thermal radiation in almost any aspect of the fluid mechanics of fires is almost entirely unknown, although its effect on the thermal characteristics of fires is the subject of many investigations. The study of large fires is hampered by the difficulty of getting good experimental data, as well as conceptual uncertainty about the intellectual boundary between large scale fire phenomena and micrometeorology. Despite three thousand years of interest in the subject, it is still not possible to quantitatively explain how a fire burns.

Detonation Research

As mentioned in the Introduction, safety considerations continue to be a major factor driving detonation research. But detonations also play an important role in such applications as supersonic combustion ram jets, hypervelocity drivers, detonative manufacturing processes, automotive engine knock, and fuel-air explosions, among others. Detonations are also central to the technology of solid explosives. The detonation of solids is a field by itself involving not only fluid mechanics and chemistry but structural mechanics as well. The detonation of solids is not considered here, but many of the results developed for gaseous and heterogeneous detonations are applicable.

The factors governing the initiation of detonations either by the sudden release of energy or by transition from deflagration to detonation (DDT), the steady state propagation characteristics, and the detonability of various fuel-oxidizer mixtures are the main targets of most detonation research. Early work has shown that the steady propagation velocity or Chapman-Jouguet (CJ) velocity of a lossless detonation in a gaseous fuel oxidizer mixture can be determined from an essentially equilibrium thermodynamic calculation without any consideration of the kinetics of the combustion reactions. Establishing the physics of initiation and of the effect of losses due to the presence of walls, obstacles or bounding compressible media requires consideration of the structure of the detonation front. The earliest proposed structure due to Zeldovitch, Neumann, and Doering (ZND) assumes that the detonation consists of a leading shock wave followed by a one-dimensional reaction zone whose structure depends on the chemical kinetics of the fuel-oxidizer mixture under consideration. Particularly for hydrocarbon fuels, the reaction zone is often dominated by an induction region during which properties remain almost constant followed by a narrow reaction zone in which the heat releasing reactions take place.

While the one-dimensional ZND model has provided a basis for estimating the effect of wall losses and the minimum energy required for direct initiation, analysis has shown that this structure is inherently unstable. The spinning and galloping detonations observed under limiting conditions certainly are not one-dimensional, and the instability of the ZND structure is supported by the experimental observation that the structure of all gaseous detonations is inherently unstable and governed by the the dynamics of the continual interaction of transverse waves propagating across the main detonation front. This structure is referred to as "cellular structure" because these interactions trace out a sequence of cellular patterns on soot covered foils placed on the walls of detonation tubes.

Deflagration transition has been observed to involve highly accelerated combustion fronts which induce shock waves ahead of them. The resultant "processing" sensitizes the combustible mixture ahead of the flame and transition to detonation occurs when a small disturbance due to turbulence or some other phenomenon causes this sensitized mixture to explode. During this initial "explosion within explosion" phase pressures are generated which are far in excess of the pressure behind a steadily propagating CJ wave. While there have been many observations and analytical studies and numerical simulations of this process, DDT is still not completely predictable or understood. A striking feature of DDT is the appearance of combustion fronts with velocities as high as 700 - 800 m/s.

The diffraction of detonation waves by obstacles, which is often involved in DDT, and the interactions between different detonating explosive media or between a detonation and a bounding inert material involve oblique detonations and other two- and three-dimensional reactive shock configurations. Such phenomena also will be involved in supersonic combustion ram jets, and are central to certain types of hypervelocity drivers and the proposed oblique detonation ram jet. It has been possible to observe some of these two- and three-dimensional interactions using Schlieren photography with exposure times as short as 10 nanoseconds and to measure the pressure signatures generated on the containing walls. There also has been some success in simulating these phenomena numerically on a qualitative basis but so far there have not been one on one quantitative comparisons with experiment.

The following items are promising research topics:

Schlieren photography and the measurement of surface pressures are the main diagnostic tools available for the study of gaseous and heterogeneous detonations. High speed optical diagnostics, which are now available, should be applied to resolve the details of gaseous detonation structure, of detonative interactions and diffraction past obstacles, and of Deflagration-Detonation Transition.

The reaction zone structure, initiation, and the propagation characteristics of spray, dust, and film detonations for various materials should be investigated in detail. Detonability limits should be established. The role of cellular structure, if any, in heterogeneous detonations should be explored.

The role of turbulence in the transition to, and propagation of, detonations in gaseous and heterogeneous mixtures should be explored in detail. The structure of the turbulence present under various test conditions needs to be carefully characterized.

The high speed combustion fronts which have been observed in DDT need to be studied in detail. The usual mechanisms of turbulent flame propagation do not provide an explanation for the high flame velocities of hundreds of meters per second observed in practice.

Heterogeneous detonations involve the ignition and subsequent combustion of fuel droplets or dust particles. Because of the sparsity of data in the microsecond range involved, data on shock induced particle and droplet ignition and combustion is lacking. These processes should be tracked in detail experimentally.

Properties of both gaseous and heterogeneous detonations, particularly in marginal cases, are strongly dependent on scale. Both large scale and laboratory scale facilities are available for studying detonation behavior. Thus, coal-mine sized facilities are available in both the US and Poland, and intermediate sized test facilities exist in many laboratories throughout the world. A coordinated experimental program, which takes advantage of all of these facilities, should be designed and carried out to determine the effect of scale on detonation characteristics under conditions which are otherwise comparable.

Although the cellular and dynamic structure of gaseous detonations has been simulated numerically using both two- and three-dimensional models, many questions remain, e.g., in some cases the results are very sensitive to the grid size used. Numerical simulation studies of the dynamic detonation structure should be continued using the more advanced computer technology now available.

Development of simulations of large scale interactions, that is on a scale larger than that of the individual detonation cells, should be continued. Such simulations should be extended to smaller grid sizes and to three-dimensional interactions.

In order to make the computations tractable most simulations of detonations and other reactive flows use simplified models for the chemistry involved. In the case of detonations a two step model is often used consisting of an induction zone followed by an almost discontinuous reaction front.

Efforts should be made to develop algorithms using full chemistry, or at least some of the partial or approximate reaction schemes currently under investigation.

Heterogeneous detonations can involve mixtures of fuel drops or dust particles with air or oxygen, of gaseous fuel-oxidizer mixtures and combustible or inert particles, or of fuel slurries and a gaseous oxidizer. Most models of such heterogeneous detonations assume a one-dimensional ZND reaction zone structure, and monodisperse droplets or particles. Such models can only serve as a rough approximation. Hence there is a strong need for extensive theoretical and numerical studies of such heterogeneous detonations.

Although DDT has been the subject of research for many years, this process is still not well understood and many uncertainties remain. Recent advances in algorithms and in computing power should be applied to the development of comprehensive simulations of DDT in both all gaseous and heterogeneous media.

Heterogeneous detonations depend on mixing of fuel in solid or liquid form with the gaseous oxidizer then followed by ignition and combustion. The physics of these processes, involving the interaction between the high speed flow behind the leading shock of the detonation and droplets or particles of various materials, is not fully understood. Modeling studies of particle flow interactions are therefore required to provide proper interpretations of experimental measurements and appropriate input for the simulation of heterogeneous detonations.

While there have been some studies of the effects of wall boundary layers on detonation propagation, many analytical and numerical studies of detonations propagating in tubes ignore this effect, a fact which may account for the divergence between theory and experiment in some cases. Boundary layers will be especially important in the propagation of detonations in small tubes and in DDT. The propagation of detonations through the small spaces and gaps in internal combustion engines is thought to be responsible for much of the damage caused by engine knock, and there viscous flows may be a dominant effect. The effects of boundary layers and other viscous phenomena on the propagation of detonations should therefore be investigated, both analytically and numerically particularly in the more complicated two and three dimensional configurations.

In conclusion, the study of detonations, particularly when heterogeneous detonations are included, requires the simultaneous consideration of high speed compressible reactive flow, two-phase flows, turbulence, boundary layers, gas-particle or gas-droplet interactions, and heterogeneous or gas-phase particle or droplet combustion. The study of detonations thus encompasses a wide range of fluid dynamic phenomena.

GENERAL REFERENCES

Bachalo, W.D. (1994) "Injection dispersion and combustion of liquid fuels" *Twenty-Fifth Symp. (Int'l) on Combust.*, The Combustion Institute, pp. 333-344.

Dixon-Lewis, A. (1992) "Structure of laminar flames", *Twenty-Fifth Symp. (Int'l) on Combust.*, The Combustion Institute, pp. 305-324.

Maly, R.R. (1994) "State of the art and future needs in S.I. engine combustion," *Twenty-Fifth Symp. (Int'l.) on Combust.*, The Combustion Institute, pp. 111-124.

Pope, S.B. (1992) "Computation of turbulent combustion: progress and challenges", *Twenty-Fifth Symp. (Int'l) on Combust.*, The Combustion Institute, pp. 591-612.

Prather, M.J. and Logan, J.A. (1994) "Combustion's impact on the global atmosphere", *Twenty-Fifth Symp. (Int'l) on Combust.*, The Combustion Institute, pp. 1513-1527.