Applications of Heat Transfer Fundamentals to Fire Modeling

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Abstract

The fire industry relies on fire engineers and scientists to develop materials and technologies used to either resist, detect, or suppress fire. While combustion processes are the drivers for what might be considered to be fire phenomena, it is heat transfer physics that mediate how fire spreads. Much of the knowledge of fire phenomena has been encapsulated and exercised in fire modeling software tools. Over the past 30 years, participants in the fire industry have begun to use fire modeling tools to aid in decision making associated with design and analysis. In the rest of this paper we will discuss what the drivers have been for the growth of fire modeling tools, the types of submodels incorporated into such tools, the role of model verification, validation, and uncertainty propagation in these tools, and possible futures for these types of tools to best meet the requirements of the user community. Throughout this discussion, we identify how heat transfer research has supported and aided the advancement of fire modeling.

Introduction

On this occasion of the 75th anniversary of the ASME Heat Transfer Division, we provide an overview of the fire industry and discuss how heat and mass transfer fundamentals are applied in fire modeling. The fire industry, which will be discussed shortly, relies on fire engineers and fire scientists to advance materials and technologies used to either resist, detect, or suppress fire. Fire, as a phenomenon, might be considered wild and untamed combustion. So, while combustion processes are the drivers for fire phenomena, the engineering of systems to address the fire's development is central to fire engineering. The fire industry is a vast enterprise that touches on many aspects of the economy. Starting with manufacturing companies, one finds that there is a supply chain that continuously evaluates how fire impacts their products. Chemicals and materials companies form one group of companies in the fire economy. These enterprises seek to deliver materials that are more resistant to thermal degradation and subsequent ignition. Manufacturers of finished products, whether consumer goods or industrial goods, are constrained in their choices of designs and materials by the effect that these choices might have on the ignition and burning characteristics of the delivered product. The construction

industry, both for residential and commercial structures, is strongly constrained through building codes to produce structures that meet underlying life safety requirements. To make the built environment safer, there are product companies that continue to innovate in fire detection, alarm, and suppression systems. While many of these technologies are intended to operate autonomously, there are also fire mitigation technologies intended for use by the fire service. In the United States alone there are over one million fire fighters who use continually improved tools and equipment to fight fire. The service component of the fire industry includes public safety personnel, research and testing organizations, standards organizations, insurance firms, legal firms, and others. For the various stakeholders in the fire economy, answers are sought on how fire affects the particular issues that they deal with.

Much of the knowledge of fire phenomena has been encapsulated and exercised in fire modeling software tools. Over the past 30 years, participants in the fire industry have begun to use fire modeling tools to aid in decision making associated with design and analysis. In the rest of this paper we will discuss what the drivers have been for the growth of fire modeling tools, the types of submodels incorporated into such tools, the role of model verification, validation, and uncertainty propagation in these tools, and possible futures for these types of tools to best meet the requirements of the user community.

Why Model Fires?

One of the primary drivers for development and use of fire models has been the growth of the fire protection engineering field. Fire protection engineering - the design of buildings to protect people and property from fire - is at the beginning of a major evolution. This evolution is moving away from designing buildings based on specific rules and towards designing based on predictions of what would happen in the event of a fire. This evolution is changing the codes and standards used to regulate building construction from "prescriptive" to "performance based." Advances in fire modeling capabilities plays a key role in enabling and facilitating this change. This evolution is not unique to fire protection engineering. Other engineering disciplines evolved in response to advances in understanding of their underpinning science. Over the past century, fields like mechanical engineering and structural engineering have evolved as new materials, manufacturing processes, and engineered systems pushed the boundaries of existing knowledge and technical capabilities. These changes facilitated innovation in those disciplines. Similarly, fire protection engineering has been influenced by improvements in the understanding of fire science and societal desire for new, cost effective, and innovative building designs.

Almost all buildings today are designed and constructed to meet the provisions of prescriptive codes and standards. These prescriptive codes and standards describe what is acceptable or not acceptable in specific terms. Fire safety provisions include what types of fire safety systems should be installed in buildings and acceptable building geometries. Most engineering design resources are expended on commercial properties, and commercial properties perform very well in fire. For example, in 2011, there were 3,005 civilian fire deaths in the United States. Of these deaths, 2,520 (84%) occurred in a home (Karter, 2012). Fire protection

engineering is generally not applied in the design of residential buildings, but is used in the development of tests for characterizing the construction materials and finished products used in a house. The economics of the fire industry are staggering. In the United States alone, direct and indirect fire costs represent approximately 2% of the GDP (Hall, 2012). These costs range from the cost of fire protection and mitigation to the additional costs of construction associated with adherence to fire safety provisions to the cost of fire losses.

Blind adherence to fire provisions that have not necessarily evolved with changes in materials, technologies, and knowledge has negative consequences. One fundamental tenet of engineering is providing the necessary level of safety at the most reasonable cost. While the buildings to which engineering has traditionally been applied have an excellent history of fire performance, they also have an unknown safety margin. Ideally, model-based fire design would be useful to assessing the marginal cost for a specified level of safety. The use of performance-based design and fire models would allow the fire protection that is provided in a building to be tailored to the characteristics of the building, the items stored within the building, and the people that would use the building.

Another fundamental tenet of engineering is to incorporate the best available scientific knowledge into tools and processes. Application of prescriptive design typically is accomplished with minimal reference to the engineering and scientific literature. This results in an unknown and inconsistent level of safety. Structural fire resistance can be used as a case study. Consider three relatively recent fires that occurred in the United States – One Meridian Plaza, Philadelphia, 1991 (Routley *et al*., 1991); First Interstate Bank, Los Angeles, 1988 (Routley, 1988); and the World Trade Center towers, New York City, 2001. In the case of One Meridian Plaza and the First Interstate Bank, both buildings withstood fires of very long duration. However, the World Trade Center towers collapsed after 102 minutes and 57 minutes of fire exposure, respectively (Milke, 2003). While the fires in World Trade Center were ignited by aircraft collisions, the bulk of the fire exposure resulted from ordinary combustible material and not jet fuel (Milke 2003). Although the fires did not start in the same manner, each of the fires in these buildings was similar in magnitude, but may have provided a different thermal load to the structural components. Regardless of the performance intended by compliance with prescriptive codes, these buildings did not all perform in a similar manner. Heat transfer processes couple the fire to the structure and should be modeled in a meaningful way for inclusion in structural performance-based design. Through a validated performance-based design process, structures could be designed such that structural fire performance would meet the needs of the community and the building owner in the most efficient means possible.

Early (pre-1900's) fire protection requirements were generally prescriptive, with such requirements as the permissible materials from which building exteriors could be constructed or the minimum acceptable spacing between buildings. It is notable that while not explicitly identified, the choice of building materials and the spacing requirements were associated with underlying heat transfer processes. Most modern building and fire code requirements more explicitly have some element of performance associated with them, which can enable the use of

fire models. Performance-based approaches for designing building fire protection can be traced to the early 1970's, when the Goal-Oriented Approach to Building Fire Safety was developed by the United States General Services Administration (Custer and Meacham, 1997). The GSA approach was developed to help the United States government evaluate fire safety in high-rise buildings. Over the 1970's, the GSA work continued to evolve, spawning the Fire Safety Evaluation System (ultimately published as NFPA 101A), the Building Fire Safety Engineering Methodology, and the Fire Safety Concepts Tree (NFPA 550).

The GSA and subsequent works were published as guidelines, meaning that they could be used as a voluntary alternative to strict compliance with prescriptive codes. In 1985, the first performance-based code was published – the performance-based British Regulations. New Zealand published a performance-based building code in 1992, and Australia followed suit in 1995. Other major developments in performance-based design include the following publications:

- First edition of the *SFPE Handbook of Fire Protection Engineering*, 1988
- *Performance Requirements for Fire Safety and Technical Guide for Verification by Calculation* by the Nordic Committee on Building Regulations in 1995
- Performance option in the NFPA *Life Safety Code* in 2000
- *SFPE Engineering Guide to Performance-Based Fire Protection Analysis and Design of Buildings* in 2000
- Japanese performance-based Building Standard Law in 2000
- *ICC (International Code Council) Performance Code for Buildings and Facilities* in 2001
- Performance option in the *NFPA Building Code* in 2003

Each of these published documents facilitated the use of fire models in the design of buildings.

Beyond the design of structures, fire models are increasingly used in forensic analyses. A fire loss may be analyzed to determine the cause and origin and contributing factors. Fire models allow the analyst to hypothesize a scenario and determine if the modeled results of the scenario are consistent with observations from the fire. Forensic analysis in fires is an extremely challenging inverse analysis process since the fire destroys much of the evidence of the factors that created it. Nevertheless, the fire leaves signatures even after consuming many parts of the structure. The National Fire Protection Association's Guide for Fire and Explosion Investigations (NFPA 921) provides guidance to fire investigation professionals to improve the overall quality of the fire investigation process. The fire investigation process is used to assess if improvements can be made in codes and standards after major losses have occurred. The process is also used in civil litigation and criminal prosecution to determine culpability when fire has caused damage, injury, or death. In the civil litigation context in the US, while insurance companies will likely issue some initial settlements, the subrogation process is used to assess

responsibility to the various parties involved in the litigation. In the litigation, fire investigators, fire engineers, and fire scientists serve as expert witnesses using their expertise in fire evolution to propose or refute various hypotheses on how some aspect of the fire took place. Experts serve in similar capacity in criminal prosecution in the US, but unlike in civil cases, a defendant in a criminal case could be given a death sentence based on evidence and witness testimony. The gravity of this consequence should require a process and standard for hypothesis testing that is as stringent as can possibly be devised. Fire models are more routinely being used in both civil litigation and criminal prosecution. There should be a path forward on how to incorporate the uncertainty inherent in any given model into a hypothesis testing standard.

Physics and Submodels

The typical structure fire in the United States takes place in a single family residence. While the most likely room for a fire to start is the kitchen, these fires tend to be more monitored than fires that begin in other parts of the home. Undetected fires often begin when a heat source such as a compromised electrical connection, unmonitored candle, or improperly discarded cigarette heats up some organic mass of material. The heat source heats the material until the material begins to pyrolyze wherein volatile material is released from it. Depending on the local flow conditions, type and arrangement of the material, and intensity of the heat source, the pyrolysis process could lead to smoldering combustion or transition into gas phase flaming combustion. If a flame develops, the flame spreads over the fuel surface in what is essentially a continuous ignition process. With increased flame spread and as more of the fuel material is consumed by the fire, the fire products and plume can begin to accumulate in sufficient concentration in the upper regions of the room that the heat transfer from this region begins to affect the overall heating rate of all fuel material within the compartment. The upper layer radiative heating increases the burning rate dramatically, if there is enough oxygen within the room. Fire models have been developed to predict the evolution of any given fire scenaro. Deterministic fire models have evolved over the past 40 years to the point where there are three basic types: empirical correlations, zone models, and computational fluid dynamics (CFD) models. The correlations were developed in the 1970s and 1980s as a combination of classical buoyant plume theory and well-stirred reactor concepts. Using estimates of the fire's heat release rate and the basic compartment dimensions and material properties, it became possible to predict average hot gas layer temperatures, sprinkler activation times, and the time to flashover (where the compartment becomes oxygen limited and engulfed in flames). These correlations are simple, robust, and remain to this day a primary component of any fire protection engineering design. However, the correlations were limited to single compartments and very simple geometries, and there soon became a need to model a series of compartments or even an entire building. Thus, in the 1980s, the two-zone models were developed. The basic idea of these models is that a fire creates two distinct thermal layers in a compartment, and pressure differences between compartments drive heat and smoke from one to the other. A zone model is essentially a stiff system of ordinary differential equations that can be solved in seconds to simulate the spread of

smoke and heat throughout a building. As zone models became widely used through the 1990s, geometrical limitations once again drove the profession towards more complex modeling tools. Computational fluid dynamics (CFD) codes were soon being developed for fire specific problems. An overview of the issues in CFD modeling of fire is provided by McGrattan (2005). With CFD, there is no need to limit the computational domain to conform to the basic two layer concept, and, thus, a much wider array of applications opened up, coinciding with the architectural trend towards unconventional building design.

Regardless of type, what distinguishes a fire model from any other type of simulation tool is the source term in the energy conservation equation; namely the fire. The fundamental physical process that drives fire phenomena is the combustion process which can occur either in the gas phase, or within a porous medium, or on the surface of a material. In the overall evolution of a fire, the gas phase flaming reaction represents only one part of the overall dynamic. Torero (2012) detailed the role of combustion science in fire safety engineering. The following discussions consider the same physical processes noted by Torero, but more narrowly discuss the roles of heat and mass transfer analysis to the overall system level modeling. The discussion also identifies the role of data reduction models, many of which require heat and mass transfer models, in advancing the theoretical bases used in fire modeling.

Pyrolysis

In fire applications, the fuel is often an inhomogeneous condensed phase material. A significant part of fire modeling is characterizing the thermophysical and chemical properties of arbitrary engineered materials. One requirement of the modeling process is to be able to describe solid thermo-chemical pyrolysis. While the chemistry and the mechanical evolution of the materials have a significant effect on pyrolysis, the amount of fuel produced is also strongly coupled to complex heat and mass transfer processes. The temperature of the material, initially at ambient, increases with convective and/or radiative heating of the material's surface. Because the radiative heat flux in fire scenarios is often larger than the convective flux, it can be important in some scenarios to properly couple the details of the radiative heat flux to the condensed phase fuel. The evolved pyrolysis products from the condensed phase decomposition may modulate the incident radiative field near the condensed phase interface. Typically, the highest temperatures will be achieved close to the surface, but energy transfer in-depth will result in a spatially and temporally varying internal temperature distribution. For some scenarios, it is important to characterize the radiative field coupling within the condensed phase. In general, however, for a decoupled analysis of solid pyrolysis, the evolution of the in-depth temperature field is modeled using an energy balance in a control volume limited by the surface of the material for which the surface energy balance sets a boundary condition.

Pyrolysis tends to be an endothermic process controlled by many chemical reactions which are strong functions of the temperature. Most pyrolysis reaction rates tend to be described by Arrhenius type dependence on the temperature. Depending on the fuel, heating characteristics, and local gas phase species constituents, the pyrolysis process can follow

distinctively different paths. Because it is difficult to in-situ sample pyrolysing materials in the same way that one can probe gas phase systems, a much less resolved picture exists of the chemical pathways. These paths can be a compendium of numerous reactions that could be sequential or compete against each other. Furthermore, the chemical pathways can be strongly influenced by the presence of oxygen (Hirata et al. 1985, DiBlasi et al, 1993). The effect of oxygen on the degradation kinetics emphasizes the importance of mass transfer effects within the material. In-depth oxygen diffusion is controlled by the structure of the solid. Some materials are highly permeable and allow unrestricted transport of species in and out of the solid. The permeability of the fuel can be a function of many variables including the degradation and consumption of the material and has deserved very little attention in the fire literature. Oxygen concentrations will be controlled by the local permeability and by production/consumption rates, thus indirectly by the temperature distribution. The effects of permeability and pressure are combined in a complex manner to define the flow within the porous fuel medium. This remains an unresolved problem.

For charring materials, pyrolysis leads to the production of gaseous fuel (pyrolyzate) and a residual solid phase char. The char is mainly a carbonaceous solid that could be further decomposed. The secondary decomposition could be complete, leading to an inert ash or to a secondary char that can be further decomposed in a single or multiple steps. Non-charring materials decompose leaving no residue behind. One approach to providing global characterization of the pyrolysis process is to apply thermal analytical methods to thermally decomposing materials.

Often, the kinetics of degradation are parameterized using experiments like thermogravimetric analysis (TGA). In TGA a sample of a material is subjected to a heating history while the mass of the sample is measured as the sample thermally decomposes. Typically, sample sizes for these materials are considered to be sufficiently small that transport time scales are fast relative to chemical decomposition time scales. Hence, the samples can be considered to be thermally and chemically lumped. By assuming that heat and mass transfer processes within the sample are fast relative to the chemical time scales, the mass loss rate is then controlled by the decomposition kinetics. Rate parameters can then be derived from the mass loss rate data, but there are concerns that such data do not adequately represent the true decomposition processes associated with heating rates associated with fires (Conesa, 1996; Burnham and Weese, 2004; Bruns and Ezekoye 2009). Additionally, as research progresses on the effects of inorganic micro and nanoscale additives on flammability, questions are being raised on the role of heat and mass transfer physics on experimental observations (Kashiwagi et al., 2005).

Other details of the decomposition process can be found from tests like differential scanning calorimetry (DSC) (Höhne et al., 2003, Stoliarov, 2008). In DSC two cells, one with a reference material and the other with the sample under consideration are heated with a prescribed temperature time history. Differences in the amount of heating required between the two samples is used to infer the effective thermodynamic parameters of the sample in question. The

data reduction model for the DSC could either be limited to the sample model or could include the furnace and reference material models. Both TGA and DSC based studies tend to produce the relevant constants for reduced chemical mechanisms that represent the complex degradation process. Given that the reaction rate is a strong function of temperature, it is clear that the adequate resolution of the energy equation is paramount in defining the degradation rates.

Prediction of evolved species from the degrading material is important in the ignition phase of a material and may be important in describing the products of flaming combustion. As in other heat and mass transfer applications, computations and models at atomic and molecular scales have begun to play an ever increasing role in characterizing physical processes. The connection between macroscopic and continuum descriptions of material evolution and atomistic descriptions has been made using modified classical molecular dynamics simulation concepts. Various flavors of reactive molecular dynamics (MD) simulation tools and techniques have evolved wherein the electronic and atomic potential energy surface modifications are included in classical MD models as submodels to describe bond breakage steps (Stoliarov et al., 2003; Nyden et al., 2004; Smith et al., 2011). Quantum chemistry calculations are performed offline using either ab-initio tools or hybrid approaches like density function theory to inform the reaction chemistry of the models (Car and Parrinello, 1985).

Because the chemical pathways leading to the pyrolysis of most solid fuels of interest in fire are unknown, many studies have sought to develop reduced chemical mechanisms for the pyrolysis of specific solids following the initial approach of Rein et al. (2006) and Lautenberger et al, (2006). Even for reduced mechanisms, there is still great uncertainty on the chemical pathways, the number of reaction steps required and the parameters associated with them. Data reduction models, used to test these mechanisms and fit the parameters, rely on complex heat and mass transfer models that are coupled with the reduced chemical degradation models containing the unknown parameters. Because of the large number of parameters and degrees of freedom that need to be explored by the optimization process, the required amount of experimental data required in the optimization process (TGA, DSC, cone calorimeter) often becomes infeasible. Even the nature of these experiments and associated uncertainty in the data propagates further uncertainty into the calibrated parameters (Carvel et al., 2011 and Rogaume et al., 2011).

At the continuum scale, fuel decomposition models should also be able to describe heat and mass transfer processes within arbitrary condensed phase materials undergoing thermal degradation. While a framework exists to model such processes using, as an example, the formalism developed for porous media heat and mass transfer (Kaviany, 1991), the details associated with characterization of thermophysical and transport properties remain a challenge. Further, it is generally unclear how to properly specify the appropriate level of complexity required in any particular analysis of a complex composite system in which there are synergistic effects between the materials due to manufacturing features etc. The coupled effects of decomposition and transport are evident when one considers the range of actual degradation behavior that potentially exists in fire scenarios. Common polymeric materials in fire environments range from thermoplastics to thermosets. There are materials that melt and drip,

while others form a char layer. These gross changes to physical configuration of the material often affect the overall evolution of the fire (Ohlemiller, 2000). At the fundamental level, melt flow depends on the temperature, morphology, and molecular weight distribution of the polymeric system (Berry and Fox, 1968). The fluid mechanics, heat transfer and materials processing literature has developed various ways to model melting and flowing polymeric systems (Denn, 1990; Jaluria, 2001). Because of melting and melt flow, a localized fire could spread by burning droplets or a flowing melt stream to other adjacent fuel packets.

Ignition

Ignition is a competition between the exothermic energy release rate and heat losses from the reacting gases to unreacted gas and to the condensed phase fuel. Obviously, a flammable mixture is required before flaming ignition can occur. Before flaming ignition can occur, a sufficient concentration of fuel vapor needs to be available in the gas phase. The solid decomposition products in the gas phase depend on many factors and might be a combination of solid phase pyrolysis and oxidation products. Thus, the product composition might include fully oxidized compounds such as carbon dioxide (CO_2), partially oxidized gases such as carbon monoxide (CO) and other molecules that can have varying levels of partial oxidation. As an example, Kashiwagi and Nambu (1992) studied the degradation products of cellulosic paper showing that there is a significant presence of inert gases like water vapor, fully oxidized gases like CO_2, partially oxidized products like CO and unoxidized species like CH_4 and H_2. There is very little data available on the degradation products of most materials relevant to fire, therefore, the mass fraction of flammable gases present in the local products of degradation is generally described by means of a global contribution of all compounds that can be further oxidized. This suggests that together with the gas phase reaction rates, the decomposition products concentration must be known to model ignition.

After pyrolysis gas begins to emerge from the fuel surface, the emerging fuel will encounter the ambient oxidizer and possibly produce a flammable mixture. Given that a complex fuel flow is migrating into the oxidizer flow, the definition of a flammable mixture region is not a simple one. In standard test methods the ambient flow is well defined but in real fires, flow fields are defined by the flames themselves and by the geometry of the environment (obstacles, fuel geometry, etc.) with the possibility of complex flow patterns. After a flammable mixture has been attained, this mixture needs to increase in temperature until a combustion reaction can occur. This process is described in great detail by Fernandez-Pello (1995). Niioka et al (1981) identify an induction time and a pyrolysis time. The pyrolysis time corresponds to the time required to attain a flammable mixture while the induction time is the time for the mixture to reach a temperature at which ignition can occur.

The amount of energy required for ignition can be associated to a Damköhler number (Williams, 1985). The Damköhler number corresponds to the ratio between local residence and chemical times. The chemical time represents the necessary time for the reaction chemistry to occur and is expressed as the inverse of the reaction rate. A critical Damköhler number for

ignition can then be established, above which a combustion reaction can proceed. This is probably the most precise way to describe ignition but it requires the full resolution of the flow and temperature fields as well as comprehensive knowledge of the kinetic constants associated to the combustion reaction. While the flow field can be resolved by means of Computational Fluid Dynamics (CFD) the chemistry of most fire related fuels still remains uncertain. Qualitative assessment of the Damköhler number for ignition has only been achieved for a few very well defined experimental conditions such as stagnation flows or boundary layers (Quintiere, 2006).

Auto-ignition in its simplest form is a competition between the exothermic energy release rate associated with oxidation and heat losses from premixed fuel charge. Data on auto-ignition is generally reported as Auto-Ignition Temperatures (AIT) which corresponds to a recorded temperature at the moment where ignition of a flame is first observed. A summary of much of the data available is presented by Babrauskas (2003). Given the complexity of the processes leading to auto-ignition, these values can only be taken as reference values that are a direct function of the specific test conditions. Generally, significant discrepancy is found in the literature with reported Auto-Ignition Temperatures varying more than 150 ^{o}C for a given material.

In practice, ignition is initiated by a pilot flame, hot gases, or hot element. From the perspective of ignition, the exposed solid surface represents not only a boundary between the gas and the solid, but also a potential ignition site. While regression rates can be very different between charring and non-charring materials, at the surface, the main difference between the two material types is the temperatures that can be achieved during pyrolysis. Carbonaceous chars in ambient oxygen environments can reach much higher temperatures than non-charring surfaces. In many cases, vigorous oxidation often termed surface glowing, can initiate gas phase ignition. The actual temperatures reached by the oxidizing char are controlled by heat transfer through the char, transpiration cooling by the fuel produced in-depth, and radiative losses from the glowing surface char.

The presence of a pilot can simplify modeling of the gas phase ignition processes and somewhat reduces the influence of environmental variables. Characterization of the flow field is still required to establish the presence of a flammable mixture and heat transfer between the hot element and adjacent premixed fuel mixture. For some global models, ignition can be assumed to occur at the moment where the lean flammability limit (LFL) is attained at the location of the pilot. To attain the LFL at the pilot location it is necessary to resolve the momentum and mass transport equations simultaneously with the surface boundary conditions.

Given a flammable mixture and an ignition source, the pyrolysis rates at the moment when the flame is established will determine if a flame can continue to exist or if the combustion reaction will cease after the premixed gas mixture is consumed. The feedback from the ignited flame will enhance pyrolysis, but usually, the relatively large thermal inertia of the solid will result in a slow response, therefore it will be necessary for pyrolysis rates to already be sufficiently large even in the absence of the flame heat feedback. If pyrolysis rates are not sufficient, the flame will extinguish and continuous pyrolysis will lead once again to the

formation of a flammable mixture and subsequent ignition. This manifests itself as a sequence of flashes that precede the establishment of a flame over the combustible solid. This process is identical to the "flash point" generally associated to liquid fuels and for solid fuels has been described in detail by Atreya (1998).

The transition between the "flash point" ignition and the established flame, which could also be named the "fire point" in an analogy with liquid fuels, deserves especial attention. The characteristics of the diffusion flame established on a solid fuel surface are defined by the flow field and the supply of fuel. The rate at which both reactants reach the flame zone defines the flame temperature and thus the characteristic chemical time. If the amount of fuel reaching the flame is small, then the flame temperature will be low and the chemical time will be long. As described above, the flow field defines the residence time. A second critical Damköhler number appears, but this time is one of extinction. This concept has been described many times explicitly in the combustion literature (Williams, 1985) but only implicitly in the fire literature. In most discussions simplifications have been assumed leading to simpler parameters that can serve as surrogates for the Damköhler number. Williams (1985) discusses a critical gas phase temperature below which extinction will occur. If the residence time remains unchanged, then extinction is only associated to the chemical time, thus can be directly linked to a critical gas phase temperature. It can be further argued that extinction is much more sensitive to temperature than to flow, thus only radical changes in the residence time need to be addressed making this criterion a robust one. A more practical surrogate to the Damköhler number is a critical fuel mass flux criterion. The concept of critical fuel vapor mass flux for ignition resembles elements of premixed flame quenching. The attainment of a critical mass flux of fuel will be the single parameter defining the flame temperature and thus the Damköhler number (Rasbash et al, 1986). Furthermore, under more restrictive conditions the critical mass flux can be associated to a critical solid phase temperature (Thomson et al., 1988).

Combustion

Once gas phase ignition has occurred heat and mass transfer processes allow the flame to creep across the fuel, this process is referred as flame spread and has been the subject of many studies in the literature. Flame spread is effectively a sequence of ignitions, therefore will not be described here. A summary of the different flame spread studies is provided by Drysdale (2011).

A flame is described by thermal and diffusive balances with extremely sensitive temperature dependent reaction terms. The characteristic length scales in flames defined only once one appropriately characterizes the thermal and mass transport thermophysical properties. Because of the disparate length scales in a practical fire scenario, the length scale ratio between a typical flame thickness and the compartment geometry typically preclude the ability to describe the flame with adequate resolution. There are many issues to address when describing the gas phase chemistry evolution in fire models. More important than the details of the flame is that a model should be able to describe the gross heat release rate which produces the density change and dilatation in the velocity field. Depending on the quantity of interest from the fire model,

this may not be the most important chemistry issue to address. Much of the hazard posed by fires is associated with the toxicity of incomplete products of combustion such as carbon monoxide, hydrogen cyanide, and soot coated with hydrocarbons (Pitts, 1995). Unlike many scenarios studied in combustion science, in fire modeling, the incomplete products of combustion, particularly CO, are non-negligible in their impact on the overall heat release rate of the combustion process. Significant amounts of carbon monoxide are produced in a typical compartment fire because of the relatively large global fuel to air ratio. Once a condensed phase fuel has ignited, the inefficient mixing of air and fuel in the fire produces copious amounts of incomplete products. Proper description of the evolving product soup requires knowledge of the chemical composition of the condensed phase fuel and its pyrolysis products. These are typically relatively large hydrocarbons that may be also bound to various trace chemicals used as flame retardants etc. Because gas phase combustion in fire is predominantly in non-premixed flames, the pyrolysis gases evolve in high temperature environments and begin to form soot. The kinetic description of soot evolution is extremely complex even for very simple fuels. One description is that polycyclic aromatic hydrocarbon molecules, formed in the pyrolysis gas mixture, coagulate to form nascent soot particles that then grow by surface addition of smaller hydrocarbon molecules and polycyclic aromatic hydrocarbons (PAHs) and by agglomeration (Frenklach, 2002; Öktem, et al., 2005) . Predicting soot evolution is extremely important in fire modeling because the radiation heat transfer in fire is primarily associated with the soot species and because soot impacts sensor activation, human visibility, and respiratory irritation. Even for relatively simple and lower molecular weight fuels, it is very difficult to predict soot volume fractions in a flame to within a factor of two (Mehta et al, 2009, Saffaripour et al, 2011). In-situ measurements have been useful in better characterization of soot evolution.

Thermal Radiation and Soot

Fire evolution and spread is mediated by heat transfer rates. In practical fire modeling scenarios, radiation is the dominant mode of heat transfer (Sacadura, 2005). If one assumes a gray gas model for the gas mixture, and uses a Planck mean absorption coefficient for typical combustion product gases, one can easily show that when the soot volume fraction exceeds approximately 1 ppm, the soot absorption coefficient is larger than the gas absorption coefficient. In most practical fire conditions the soot volume fraction is much larger than 1 ppm in most of the fire. An exception to this rule is very near the surface of a liquid fuel pool. Because the fuel vapor has not necessarily had time to breakdown into soot, there is an abundance of fuel vapor that participates with the incident radiation. It is in this near surface region that a gray gas model might be most limited. Work in the heat transfer literature has been useful in parameterizing fuel spectral absorption coefficient models (Fuss et al, 1997). The spectral details of the absorption coefficient and its modification of the radiative intensity determine the true incident flux on the fuel surface. Depending on the interface's radiative properties, these spectral effects could be important.

Typical measurements used to characterize the soot properties are laser based extinction experiments and laser induced incandescence experiments. Both extinction and LII measurements are grounded in heat and mass transfer fundamentals. Considerable effort has gone into developing detailed descriptions of soot morphology with a goal of better characterization of the soot radiation properties and soot transport physics. Sorensen and co-workers (e.g., Cai et al, 1995), Faeth and coworkers (e.g., Köylü and Faeth, 1994), and Mulholland and coworkers (Zhu et al., 2000) characterized the mass fractal and optical properties of soot aggregates. The morphological characteristics of soot aggregates somewhat modify their radiative emission properties but do not markedly change the absorption properties if reasonable approximations are made about the soot primary particle size and volume fraction. These changes in radiative properties are neither significant for measuring soot volume fraction by extinction nor for simulations of most compartment fires. Where these morphological effects do matter is in models for smoke detection systems. Smoke detectors sense smoke using either optoelectronic or mobility principles. In both cases, the morphological properties of the smoke play a role in the detection sensitivity. A model for the radiative scattering processes in smoke detector activation was reported by Upadhyay and Ezekoye (2005), and the role of soot fractal dimension on detector processes was discussed. For LII, Knudsen number effects on the cooling rates and subsequent interpretation of LII signal outputs have been useful in validating experimental techniques (Daun et al, 2007).

While soot primarily absorbs thermal radiation, water droplets from sprinkler and mist fire suppression systems scatter radiation. From a fire design perspective, water sprays/curtains are sometimes used as radiation shields. The heat transfer submodel in a fire model should be able to model droplet scattering physics (Dembele et al., 1997). Depending on the characteristic length scales of the droplet cloud, particles can either be modeled using either a Rayleigh limit or a geometrical optics limit. For intermediate scales, full Mie analysis may be required, but approximations are often made in the specification of the phase function Additionally, the effects of both water vapor and water droplet size distribution may be included in the analysis as was done by Dembele et al.

Turbulence radiation interactions have been investigated in the literature to determine if including improved estimates of temporal and spatial temperature fluctuations affects radiative heat transfer predictions (Li and Modest, 2002). The nonlinear dependence of radiative intensity on temperature implies that for some applications, there will be significant deviation between the temporally and spatially averaged radiative emission relative to estimates based on the temporally and spatially averaged temperature.

In depth radiative transfer in some materials, particularly many polymer systems, has been shown to affect the thermal degradation and ignition characteristics of the material. As an example, Bal and Rein (2011) recently noted the importance of including in-depth radiation modeling to properly predict the ignition time of polymethylmethacrylate using a thermal ignition model. Thermal radiation induced damage and heating has also been important to characterize and analyze in the development of increasingly burn resistant protective garments

for firefighters and warfighters. Mell and Lawson (2000) applied heat transfer fundamentals to characterize the mechanisms controlling the protective properties of firefighter personal protective equipment.

Smoke and Convective Heat Transport

Fire modeling has contributed to and borrowed from developments in computational fluid dynamics in developing gas phase flow models (McGrattan, 2005). In many respects, this is one area in which fire modeling has the strongest validation. While the turbulent flow processes can be quite complex and involve variable density and composition, there is an underlying physical model (i.e., Navier Stokes) that describes the flow evolution over a range of scales. The challenge in this area of modeling is in developing submodels for physics that occur at scales smaller than the computational grid. Fire gas phase flow modeling typically takes place in compartments with characteristic length scales on the order of meters. Dissipative length scales (whether Batchelor or Kolmogorov) are often millimeter or sub-millimeter for the velocities encountered in compartment fires. It is currently infeasible to simulate processes across the range of scales. There are many approaches to modeling subgrid scale mixing in CFD, but fire modeling has traditionally looked to the meteorological literature because of its emphasis on low speed, buoyancy-driven flow (Smagorinsky, 1963; Deardorff, 1972; Germano *et al*., 1991).

Structural Response

Structural components can be compromised either by high heat fluxes or by oxidative damage. It is necessary to be able to couple the combustion evolution with descriptors of structural evolution. The overall time scales over which structures evolve are considerably longer than the time scales associated with the flow processes. On the other hand, the spatial resolution required to model structural component thermomechanical evolution is at much more resolved scales than what is typically available from fire simulation. As such, sensible ways of coupling the fire flow evolution to the structural evolution are necessary. For many scenarios, the structural evolution can be decoupled from the fire flow evolution. There are, however, scenarios in which fire induced changes in the structure strongly modify the evolution of the fire. One obvious case in which the fire affects the structure which in turn affects the fire is window glass failure. As already noted, fuel loads for typical fire compartment scenarios are globally rich. In the fire literature, the resulting fires in such compartments are said to be ventilation limited. For ventilation limited fires, the heat release rate within a compartment is controlled by the oxygen mass flow rate into the compartment. Thus, a change in the availability of oxygen entering the compartment associated with a window breaking or a door being opened dramatically impacts the fire evolution. Time scales over which a door might be breached by a fire are considerably longer than the times required to fail a window. Simple models are available for window breakage that rely on the heat transfer rates to the window, the geometry and constraints on the glass (Cuzillo & Pagni, 1998). Given the variability in window types, age, and condition, one can perhaps only view such models as being statistically descriptive. Glass breakage models rely

on thermomechanical models for the glass and window system. Glass heating by convection and radiation is important to the overall model. Details like the insulating properties of the window cladding strongly affect the crack growth and propagation. Initial microscale features of any particular glass sample provide a state of stress on the boundaries (e.g, associated with the glass being cut) and in the interior that affect breakage. In spite of this complexity, it is extremely important to provide a means for implementing window/glass breakage into fire models because of how dramatically such failures affect the subsequent fire evolution.

A slightly simpler problem is the modeling of the behavior of structural systems in fire. In this case, the potential of a structural system to affect the nature of the fire is only as a thermal boundary condition until major structural collapse (usually late in the fire evolution) occurs. By exploiting the time scale differences, one can decouple the gas phase evolution and the solid phase and the fire becomes only the forcing for the heat transfer to the solid mechanics models (generally finite element models) that are normally used to establish the evolution of a structure (Usmani et al. 2001). Interestingly, the detailed mechanical properties of common building materials are not well known at elevated temperatures associated with fire (Hu et al, 2009).

To be able to define the temporal and spatial evolution of a structure during the event of a fire, the following issues need to be resolved:

1. The temporal and spatial evolution of the gas phase fire thermal, flow, and species fields should be known.
2. The evolution of the gas phase fields determines the temporal and spatial evolution of the heat exchange between the structural elements and the gases.
3. With thermal boundary conditions defined on the structural elements, detailed analysis can then take place for the structural elements. For materials like steel the transient energy equation consists only of heat conduction and enthalpy terms with variable thermal properties, but for other more complex materials such as concrete or plaster board, complex mass transfer equations need to be resolved to account for the vaporization enthalpy as well as moisture migration.
4. The spatial and temporal evolution of the temperature of the structural elements affects the material and mechanical properties of the solid which determine stresses and deformations within the structure.
5. The results of these calculations can be used to establish quantitative failure thresholds.

The comprehensive formulation of the problem requires the coupling of the gas and solid phases. Explicit finite element models coupled with transient CFD models become a necessity if the complete interaction is to be resolved. Despite many attempts to do this, there is currently no combination of models that solves the coupled effects of fire and structure. Furthermore, there is currently no CFD model that comprehensively resolves the fire at the necessary scale and with full detail. Finite element models are more advanced but many of the mechanical and thermal properties that serve as inputs are still unavailable.

Numerous alternative approaches can be found in the literature, some of them are well argued simplifications that use the characteristics of the problem to either relax the coupling between gas and solid phase or simplify certain terms of the equations. Among these simplifications are simplified connection models, constitutive property models, total heat transfer coefficients and spatial and temporal averaging of the gas phase. These simplifications take advantage of the very different time and length scales of the solid and gas phase problems to decouple and simplify many of the processes. When correctly argued these approaches are perfectly valid and provide a true assessment of the performance of the structure as well as quantified error bars linked to uncertainties and simplifications (Buchanan, 2002).

The equations used in simple numerical methods are derived from simplified heat transfer approaches. For example, a quasi-steady-state, lumped heat capacity analysis can provide the temperature rise of unprotected steel members, while for protected steel members, the thermal resistance provided by the insulating material can be accommodated by empirically derived correlations (c.f. the Structural Eurocodes methodology (CEN, 2005)). These approximate methods allow the designer to use any appropriate gas-phase temperature-time curve, but their generality remains uncertain.

Advanced models based on numerical heat transfer methods provide a more general approach and are becoming increasingly popular both in a research and industrial context (Cox and Kumar, 2002). Their advantages lie in the ability to define an arbitrary gas-phase boundary condition and to perform conjugate heat transfer calculations in which the surface temperature is obtained from the balance of the gas- and solid-phase thermal conditions (Patankar, 1980). The analysis is typically performed in three-dimensions, thereby overcoming the limitations of simpler approaches which consider only the in-depth direction. There is a significant challenge in achieving sufficient grid resolution within the solid, where much smaller cells are normally required due to the steep thermal gradients, especially when structured meshes are adopted (which may demand a similar cell size in the gas and solid phases) (Kumar et al., 2005); this can be overcome using unstructured meshes, or by coupling to an independent high resolution mesh within the solid, though in the latter case there will still be limitations associated with the resolution of the surface cells, e.g. where these are not able to fully resolve the details of the geometry, such as an I beam. In addition, temperature-dependent properties can easily be incorporated into the calculations for greater accuracy.

The resolution of the thermal gradients is necessary to model structural behavior in fire. Without precise thermal gradients phenomena such as connection behavior, thermal expansion, thermal bowing or tensile membrane action cannot be reproduced. These phenomena determine the evolution of the structure as it is being heated and allow identifying potential forms of failure (Usmani et al, 2001). Furthermore, the potential for concrete spalling is strongly defined by temperature gradients.

A second approach that is equally valid is that of establishing a series of constraints in the form of codes and standards. These constraints guarantee a simplified environment that can be quantified by means of a simple representation. The most common of these code based

constraints are the requirements for compartmentalization. By reducing all buildings to a summation of standardized compartments, the evolution of the fire can be reduced to an energy balance and thus both gas and solid phase behavior can be deeply simplified. This particular approach still provides a true assessment of performance. The error bars, in this case, are linked to the simplifications of the physical models defining the gas and solids but also to the deviation of the real compartments from the standardized ones (Thomas and Nilsson, 1973, Harmathy, 1981)

An approach that is acquiring popularity is that of using simplified models coupled with probabilistic estimations of error. These methods, based on theories of risk and reliability, are only valid if the representation of the physical phenomena incorporates in a correct manner all the necessary variables and couplings and the probabilistic distributions for all poorly defined properties are available. In this case a probabilistic distribution of true performance can be established.

A final method is the relative assessment of performance. This method creates a realistic scenario and assesses the performance of a system against it. The realistic scenario can be a standardized temperature vs. time curve, a parametric temperature vs. time curve to provide a relative performance of a structural component or system but also a standardized compartment to assess the relative severity of a fire given different fuels. While this approach can be used for the purpose of understanding or for classification, it will never provide true performance assessment.

Human Behavior and Egress

Modeling human activity in fires has primarily considered the effects of fire on civilian occupants within structures. The type of civilian action in fires that has been most examined has been egress modeling, where the time necessary to evacuate a building is predicted (Gwynne, 2001). One of two different approaches is used in an egress model: either (1) predicting occupant movement speed by using a hydraulic analogy, or (2) assigning each occupant its own behavioral characteristics. The hydraulic analogy predicts movements speeds based on the width of the egress component and the density of occupants within that component. Behavioral models rely simple rules based upon the location of exits, amount of heat or smoke, and assumed mobility data to characterize the evacuation of a structure. Building occupants can affect the fire conditions in a building by actions such as opening doors, windows etc. Similarly, firefighters affect the fire by changing the ventilation in the structure and also by application of water and other suppressants to the fire. However, the effects of occupants or the fire service on the progression of fire are generally not modeled. There is an opportunity for coupling egress models with fire simulations to improve the quality of simulation and support firefighting training and post incident reviews.

Modeling Engineering Subsystems

The range of engineered systems that are frequently encountered in compartment fires has motivated the development of submodels for heating ventilation and air conditioning systems

(Gaunt, 2000), sprinkler activation (Heskestad and Bill, 1988), and smoke detection (Cleary *et al*., 1999). Typically, these submodels are in the form of an ordinary differential equation involving a handful of empirical parameters. Ideally, these parameters are obtained via a standard test, like the RTI (Response Time Index) of a sprinkler.

In addition to fire protection and building systems, models of measurement devices are commonly added to fire models. For example, gas temperatures are typically measured with bare-bead thermocouples which do not actually measure the true gas temperature but rather the small bead of metal itself. A fire model can easily incorporate simple models of a thermocouple (Welsh and Rubini, 1997) so that model predictions can be compared directly with measurements for validation purposes. Another useful measurement device that can be easily modeled is a plate thermometer, a thin, insulated inconel plate useful for monitoring standard furnace tests (Wickström *et al*., 2007). These simple models of measurement devices help the model user to report the computed quantity in a way that an experimentalist would so that there is less confusion when comparing model and experimental results.

Model Verification and Validation

The use of fire models currently extends beyond the fire research laboratories and into the engineering, fire service, and legal communities. Sufficient evaluation of a model is necessary to ensure that users and regulatory authorities can judge the adequacy of its technical basis, appropriateness of its use, and confidence level of its predictions. This is ever more true due to the emergence of performance-based design as an alternative to prescriptive regulations.

The model evaluation process consists of two main components: verification and validation [ASTM E 1355]. Verification is a process to check the correctness of the solution of the governing equations. Verification does not imply that the governing equations are appropriate, only that the equations are being solved correctly. Validation is a process to determine the appropriateness of the governing equations as a mathematical model of the physical phenomena of interest. Typically, validation involves comparing model results with experimental measurement. Differences that cannot be attributed to uncertainty in the experimental measurements are attributed to the assumptions and simplifications of the physical model.

Consider in turn the three basic classes of fire models. Empirical correlations are typically presented in the form of simple formulae or equations that require, at most, a spreadsheet program to calculate a result. Verification of such models is trivial. Validation is often assumed, given that the models are typically based on full-scale experiments. However, there have been efforts in recent years to compare classic empirical correlations with experiments that were not used in their original development. One study, sponsored by the United States Nuclear Regulatory Commission and the Electrical Power Research Institute [Hill et al. 2007], considered a number of classic compartment fire correlations and found that these correlations tend to over-predict compartment temperatures. This result is looked upon favorably by regulatory agencies who prefer that these simple models err “on the conservative side.”

Next, consider two-zone models. These models are essentially a set of ordinary differential equations for the average upper and lower temperatures and pressures within a set of compartments. Again, verification of the governing equation solver is straightforward, and this procedure is supplemented by global checks of mass and energy conservation within each "control volume." Validation of zone models has traditionally consisted of comparing model predictions with the results of full-scale experiments in compartments that conformed to the basic assumptions of the model; that is, relatively flat, unobstructed ceilings and simple geometries. More recent validation work [Hill et al. 2007], however, has documented more challenging fire scenarios that highlight the strengths and weaknesses of these models.

Finally, verification and validation of CFD fire models has dominated this area in the past decade. Neither is trivial. Verification of these models takes on many forms, from grid resolution (convergence) studies to checks of the conservation laws of mass, energy and momentum. Validation of CFD models is similar to that of the simpler models -- comparisons with full-scale experiments. Given the abundance of fire test data, it is more practical to compare model and experiment rather than to dissect the model into its constituent parts and evaluate each separately using various analytical techniques. For other fields of CFD, this is unavoidable, but for obvious reasons fire science has yielded a wealth of test data with which to evaluate the models. In addition, regulatory authorities are typically not experts in CFD and prefer simple comparisons of model predictions with experimental measurements as a means of assessing the accuracy of the model.

So what are the challenges associated with fire model V&V?

1. Even though there is an abundance of fire test data, many of these past experiments were not intended for model validation. This means that the experiments are not well-documented, experimental uncertainties are not reported, and the test results are often presented as simple pass/fail judgments with limited data to use for model validation.
2. Experiments conducted prior to the advent of oxygen consumption calorimetry do not provide accurate measurements of the fire's heat release rate. Without this key input parameter, these experiments can only serve as a rough qualitative check of the model.
3. Model validation cannot be static; that is, with each new version of the model, developers need to re-run and re-document the results of the V&V studies. From a regulatory standpoint, if a particular version of the model has been validated, this is the version that shall be used until a new validation study is performed. To address this problem, a substantial repository of validation data is being collected and archived at NIST and an automated procedure has been developed to continually re-run a suite of V&V cases so that model users can cite up to date estimates of model uncertainty.
4. Standards like ASTM E 1355 do not explicitly state how the results of model V&V studies are to be reported, and it does not specify what level of accuracy constitutes "validation." It is left to the model user to decide how to report the results of the study, and it is up to the AHJ

(Authority Having Jurisdiction) to decide if the model is appropriate for the given application. In the NRC/EPRI fire model validation study [Hill et al. 2007], the NRC and interested industry and research collaborators developed a relatively simple methodology for reporting model uncertainty. In brief, for a given model and given predicted output quantity, there is a reported relative bias and relative standard deviation that is based on comparisons to a wide range of full-scale experiments. This methodology has been applied in various ways over the years and it is now typical for a validation study to conclude that Model X over or under-predicts Quantity Y, on average, by Z %, with a relative standard deviation of sigma %.

5. From the discussion above, it is apparent that there are fairly well accepted methods for performing model V&V. These methods, however, only quantify *model uncertainty*; that is, the uncertainty in the model prediction due to assumptions and simplifications of the model itself. The issue of *parameter uncertainty*, the uncertainty related to the input parameters, is receiving more attention for two reasons: First, as models become more accurate, the relative contribution of parameter uncertainty to the overall uncertainty increases. Second, the increased use of CFD means that conventional techniques for propagating parameter uncertainty are now much more difficult to apply. Empirical correlations and to some extent zone models lend themselves nicely to the various analytical methods to assess the influence of input parameters on the resulting prediction. CFD does not because these models incorporate more detailed physics and require hours or days of computational time. Adjoint based models are gaining acceptance in many areas of CFD, and such models are likely to be incorporated into fire modeling such that sensitivities can be extracted in computationally efficient ways. In evaluating the uncertainties in model parameters, there are many ways that parameter inference can be performed. One approach gaining favor is the use of Bayesian inference in parameter estimation (Tarantola, 2005). The Bayesian formulation naturally leads to the specification of a probability density function in the parameter being evaluated (Upadhyay et al., 2011). Knowledge of the statistical distributions of the uncertain parameters provides a basis for propagating said uncertainties through the fire model to determine a risk informed quantity of interest (Upadhyay and Ezekoye, 2008).

Based on this list of challenges, there are a number of potential areas for future research. First, consider the need for experiments. There exists a considerable number of experimental data sets in which the temperature, heat flux, species concentrations, and other quantities are measured within a compartment with a controlled fire, usually a gas or liquid fuel spray burner whose heat release rate is accurately measured. These experiments are ideal for assessing the capability of the models to transport and distribute the heat from the fire throughout the compartment. What is lacking are carefully designed experiments in which the fire's heat release rate is not a specified input parameter, but rather a predicted output quantity. The most obvious example is a room filled with furniture, and certainly many experiments of this type have been conducted for various reasons, but the results of these experiments are not particularly useful for model validation because the material properties are typically not measured. Even if they are measured, to some extent, the uncertainty related to the prediction of the heat release rate of a growing, spreading fire overwhelms all other sources of uncertainty to the point where the model

at best makes a very rough qualitative prediction of the outcome. What is needed are a series of experiments of increasing complexity that can be used to assess the model capabilities step by step -- first, how well the model predicts the burning rate of a given object, second, how well the model predicts the spread of the fire from object to object, and finally, how well the model predicts the transition from small fire to flashover and beyond. Combining all of these phenomena into a single experiment does not allow for a systematic assessment of the sub-models that are adequate and those that are not and need improvement. A key component of this analysis is the propagation of parameter uncertainty. The rate of fire growth and spread is very sensitive to the material properties -- temperature-dependent thermal conductivity, specific heat and density; the choice of reaction mechanism and associated parameters; geometric complexity of the burning object.

Inverse Analysis

Inverse analysis generally refers to analysis in which the usual ideas of causality are reversed. In the heat transfer literature there has been a large body of work on development of computational techniques for inverse analysis (Beck et al., 1985; Ozisik, 2000). These approaches have been applied to parameter estimation, boundary condition estimation, and source estimation. One can arrive at an inverse solution either through an optimization process in which one seeks to minimize an objective function, defined as the difference between a forward model and some measured or desired. Alternatively, one can formulate a model in an inverse sense and use one of many approaches in the literature to generate the solution. Typically, problems formulated in an inverse sense are mathematically ill-conditioned. For problems developed as a system of equations as might be generated from differential operators or from Fredholm integral equations, an ill conditioned system is identified by the ratio of the largest to smallest singular value for the system (Hansen, 1987). Hansen discusses several approaches to regularization of the system of equations such that meaningful solutions that are less sensitive to measurement noise can be computed. Optimization based inverse analysis has been applied to problems of interest in fire scenarios (Richards et al, 1997, Jahn et al, 2011, Overholt and Ezekoye, 2012). In each of these studies, the authors used forward models for fire evolution to predict compartment fire behavior. Fire researchers at the National Institute of Standards and Technology, among others, have begun to frame a discussion on the use of building fire sensors with very fast computational models for fire for fire growth modeling for firefighter operations (Evans,2003 ; Jones et al., 2001).

Measurement systems for fire systems have also benefitted from inverse analysis techniques. Boundary condition estimation techniques for conduction analysis have been useful in development of heat flux measurement gauges in fires (Lam and Weckman, 2009). In the heat transfer literature, much of the source estimation and boundary condition estimation analysis has occurred for temporally evolving physical systems. Approaches like that of Erturk et al (2002) may be useful in better characterization of furnaces used to characterize material fire resistance and in development of fire detection analysis.

Forensic analysis in fire scenarios challenges the limits of inverse analysis techniques. For such problems, the fire often has destroyed much of the evidence associated with its evolution. The National Fire Protection Association's fire investigation reference document (NFPA 921) details the types of signatures that fire forensic analysts should consider in determining the cause and origin of a fire. These so-called fire-patterns include burn patterns on walls, depth of char on wood, spalling of concrete or masonry, glass breakage location, and other damage indicators. Many of these damage processes are thermally mediated, and any model based reconstruction of the fire should be able to predict the observed damage. The implication is that there should be available submodels to predict fire damage assessment as part of the hypothesis validation steps in forensic reconstruction.

Conclusions

Fire modeling represents a broad set of tools at various scales, with different underlying physical models used to design materials resistant to fire, model fire testing equipment, and predict fire ignition, spread, and damage in the built environment. Proper characterization of heat and mass transfer processes is critical to the predictive capability of these tools. In this paper, we have outlined different ways in which ongoing heat and mass transfer research plays a role in advancing fire models.

Several critical areas of research are evident to advance fire models. Perhaps the greatest current need in fire modeling is the need to be able to reliably predict burning rates of real materials. To do so is an interdisciplinary endeavor that requires a more nuanced view of the coupling of experiments and testing with modeling. At the heart of this endeavor is the need for improvements in condensed phase materials evolution models. Such improvements have many possible side benefits including closer integration in use of tests and models for product design. Translation of inverse modeling approaches to fire scenarios could revolutionize fire arson investigation. Fire investigation had traditionally been conducted by nontechnical investigators. Given the potential disastrous impact of an incorrect fire evolution hypothesis being accepted, the need to improve this capability is evident. Development of a fire inverse analysis framework is another interdisciplinary endeavor that will require closer coordination between experimental and computational research. On the computational and modeling side, the largest computational effort for smoke and heat transport or forensic analysis or any compartment scale analysis is the computational fluid dynamics model. Development of low dimensional models for fire flow processes would significantly improve the ability to make multiple runs for either design or forensics applications. As the overall predictive reliability of fire models improve and computing power increases, one envisions routine use of fire models to aid evacuation and firefighting operations during fire hazards.

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