CARBON MONOXIDE PRODUCTION AND PREDICTION

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ABSTRACT

A long-term research plan has been formulated which is designed to improve the understanding of and predictive capability for the formation of carbon monoxide in enclosure fires. The current understanding of the problem is briefly discussed. Goals (milestones) for the project are listed and the research plan is discussed in terms of eighteen individual research components.

1. INTRODUCTION

One of the mandates of the Center for Fire Research (CFR) is a reduction in the number of fire deaths and injuries. To achieve this goal, CFR has led the effort to characterize and model fire behavior. The development of realistic fire models allows strategies to be developed for ameliorating its effects.

Investigations have shown that a large percentage of fire deaths and injuries can be attributed to products of incomplete combustion. Even in cases where burn injuries and death occur, incapacitation of victims by fire gases often plays a pivotal role since escape from flames is hindered or rendered impossible. Careful studies (e.g., [1,2]) have shown that more than one half of all fire victims have fatal levels of carboxyhemoglobin in their bloodstreams.

Even if a complete understanding of the physiological effects of CO (in combination with effects due to other fire products, e.g., reduced oxygen and increased respiration resulting from elevated carbon dioxide concentrations) is available, accurate predictions of fire toxicity require reliable estimates for the concentrations of toxic gases generated by a fire.

Systematic investigations of CO formation in fires date from at least the 1960s. However, despite nearly three decades of research the current understanding of CO formation in enclosure fires must be characterized as poor. For any given fire scenario it is impossible to predict accurately the concentrations of CO which will be produced and transported from the room of fire origin. As a result, models for fire toxicology are dependent on crude estimates for the CO concentrations generated.

CFR has embarked on a long-term effort to develop an improved understanding of the chemistry and physics responsible for the generation of high levels of CO and the development of reliable algorithms for predicting the CO levels generated by fires. During the past year a research plan has been drafted [3] which is designed to provide the understanding necessary for the prediction of CO levels generated by enclosure fires. This presentation briefly describes the current understanding concerning CO formation in fires and the research approach which has been adopted. Goals for the project are discussed. The project plan consists of a number of research components which are included in tabular form.

The research plan has been developed following an extensive review of the existing literature and relevant intramural and extramural CFR research programs. An important component of this review is the findings of a <u>Workshop on Developing a Predictive Capability for CO Formation in Fires</u> which was held in Clearwater, Florida on December 3-4, 1988. Leading experts in the field have provided recommendations and justifications for the principal areas in which research is required in order to achieve the ultimate project goal. An executive summary of this workshop is available [4].

2. CURRENT UNDERSTANDING

Numerous large-scale enclosure fire tests have been reported in which CO concentrations have been measured (e.g., [5,6]). These tests show unequivocally that CO concentrations high enough to be life-threatening often occur in this type of fire. On the other hand, no systematic investigations of CO formation in full-scale tests have been identified in the literature, and the conditions necessary for the generation of high levels of CO are not well characterized. The uncertainties are compounded by variations in experimental protocols (e.g., probe placement) and the utilization of inadequate experimental instrumentation.

In general, high CO concentrations are associated with either smoldering or underventilated fires. Smoldering fires will not be considered here. Some crude correlations of CO formation and the ventilation parameter for an enclosure (Ah¨) have been attempted [7]. However, the fire behaviors in these studies have not been adequately assessed, and the utility of these correlations for actual fires is limited.

For locations removed from the room of origin, CO concentrations may depend critically on whether or not additional combustion of product gases occurs after exiting the enclosure. The understanding of this process is very poorly characterized, and the controlling parameters have not been identified.

Dr. George Mulholland has developed a zeroth-order model for CO formation in room fires [8] which assumes very low concentrations of CO for preflashover conditions and significant CO concentrations for postflashover fires. CO concentrations following flashover are estimated to be 0.5 times the carbon dioxide concentration. This model is based on measurements recorded in three series of full-scale fire tests performed at CFR.

In recent years some carefully performed experiments have been carried out which offer the promise of an improved understanding of CO formation in terms of engineering correlations. Workers at Harvard [9] and Cal Tech [10] have generated controlled two-layer combustion systems which closely mimic the simple two-layer model often used to represent enclosure fires. Note that, in general, these experiments are steady state while actual fires are highly dynamic. A remarkable finding of these experiments has been that the major products of combustion (including CO) for a given fuel can be correlated in terms of the global equivalence ratio in the upper layer containing the combustion products. The correlations do depend on fuel type. Experiments [10] have shown that the same correlations hold even for the cases where additional air is injected into the upper layer.

Very recently, the Cal Tech workers have extended their studies to an experimental configuration where the entire flame is located within the upper layer [11]. For this case, burning occurs entirely within a vitiated atmosphere. The rather surprising observation (based on earlier speculation in the literature) is made that very low concentrations of CO are measured for increasing fuel equivalence ratios up to the point where oxygen concentration in the vitiated environment (≈ 13%) is insufficient to support combustion. Similar observations have been made at CFR for preliminary measurements in a cone calorimeter modified to allow partial vitiation of the air supply. These studies indicate that vitiation of the air supply is not responsible for high levels of CO as long as sufficient oxygen is available for complete, fully-involved combustion.

3. PROJECT GOALS

The general project goal for the CO Production and Prediction project "is to improve the understanding of and predictive capability for the formation of carbon monoxide (CO) in fires" [3]. Clearly this overall goal is far too general to serve as a legitimate means for project planning. More specific goals (milestones) have been formulated. The following milestones represent realistic goals for a five-year research program. A five-year period has been chosen only for planning purposes. The actual project length will be dependent on resources and personnel available for the project.

1. By the end of the third year of the project an engineering correlation for CO concentrations in terms of the global equivalence ratio will be available for incorporation into fire computer models. Further work during the final two years of the project will be required to fine tune this correlation and determine the appropriate conditions for which its use is valid. By the end of the five-year period it will be possible to incorporate the effects of the combustion behavior of products exiting an enclosure on CO formation.

2. By the end of the five-year period the fundamental portion of the project will have identified the important parameters controlling CO formation in fires. A general understanding of the reasons for the success of the global equivalence ratio concept in terms of the combustion behavior within the fire plume will have been attained. Modelling of CO formation for very simple systems (e.g., a single gas burner located in an enclosure) will be possible.

4. PROJECT PLAN

A project plan has been formulated to meet the milestones listed in the last section. The plan incorporates the findings of the workshop [4] as well as the analysis of the project manager. The plan is summarized in terms of the eighteen research components listed in Table 1. The full research plan [3] describes the assumptions which went into the choice of these components in more detail.

Research component 4 deals specifically with the first milestone listed in the last section. A number of the other research components are designed to feed information into this effort. Most important are numbers 2, 9, 10, 14, 15 and 16. For planning purposes it has been assumed that a suitable engineering correlation will become available during the third year of the project, and component number 17 is included for the incorporation of the correlation into whichever fire model(s) is deemed appropriate.

In developing project goal 1 it was recognized that even though it should be possible to formulate an engineering correlation for CO concentration in terms of the global equivalence ratio within the first three years of the project, certain aspects of the problem can not be completed within this time frame. The burning behavior of gases exiting the enclosure is sure to be one of the remaining uncertainties. Components 11 and 12 are to address this problem. It is anticipated that a sufficient understanding of the controlling parameters will be available to allow crude estimates of the effects of such burning on the CO concentration correlation.

The second goal of the priority project deals with fundamental aspects of the problem. As was true for the first goal discussed above, several of the research components address this goal.

Research components 1, 2, 6, 7, 8, 9, 10, and 13 are required to generate the research findings to meet the fundamental project goal. Components 1, 2, 7, 8, 9, and 10 will aid in the identification of the important physical processes responsible for the formation of high levels of CO during ventilation-limited burning. Note that 2, 9, and 10 are also necessary to validate the engineering correlation developed to meet the first goal of the project.

In order to have confidence in the engineering correlation which is generated, it is necessary to have some understanding of the physical basis for the success of the correlation. The fundamental studies mentioned in the last paragraph will provide the insights required to develop this understanding. At the same time, component 13 deals specifically with the question of whether or not the high levels of CO formed during vitiated burning can be understood simply in terms of turbulent combustion processes. Turbulent combustion modeling is to be employed for this purpose. Note that the experimental results of component 1 are required as input for this research.

The final goal of the fundamental studies is to develop a model capable of predicting the time development and concentrations of CO for a simple prototypical fire in an enclosure. Research component 5 deals specifically with this topic.

5. FINAL COMMENTS

The complexity associated with CO formation and prediction in fires precludes an effective project by one or even a few individuals. As mentioned in Section 2, the current understanding of CO formation is very poor despite the availability of many uncoordinated investigations. The amount of expertise required to make meaningful progress and the complexity of the problem requires that a large number of research problems be addressed and that investigators have a wide range of capabilities. This is reflected in the range of research components included in Table 1.

One of the most difficult aspects of the proposed research effort will be the coordination and direction of the various components. A great deal of effort will be required on the part of the project manager to stay apprised of progress on the various efforts. The importance of project management is emphasized by including it as one the components in the research plan (Component 18, Table 1).

The research plan which has been formulated builds on existing research efforts within CFR. By utilizing these existing research components (with some redirection) along with selected new research efforts, it has been possible to formulate a research plan which brings significant resources to bear on the problem of CO prediction without requiring unreasonable levels of new funding. It seems likely that significant progress will be made if this research plan is implemented.

6. REFERENCES

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TABLE 1

#	RESEARCH COMPONENT	FUNDAMENTAL OR ENGINEERING	GOALS AND/OR PURPOSE	EXISTING RESEARCH OR NEW START	DURATION AND PROJECT TIMING
1	Study of underventilated laminar flames	Fundamental	To characterize the structure of underventilated laminar flames and to correlate chemical species in terms of the local equivalence ratio	New start	Years 1-4
2	Laboratory studies of turbulent underventilated flames	Engineering	To characterize structures of underventilated turbulent fires and to test the validity of the global equivalence ratio concept for correlating major gas species in upper layers	Existing	Years 1-3 Years 1-4
3	Development of experimental flame diagnostics	Both	To develop and test techniques for accurate flame gas (particularly CO) measurements within sooting flames	New start	Years 1-2
4	Develop and test global equivalence ratio concept for predicting CO in fires	Engineering	To develop the global equivalence ratio concept to allow prediction of CO in actual fires and incorporation into CFR fire models	New start	Years 1-5
5	Prediction of CO for simple configuration of burning in enclosure	Both	To develop fundamental modeling capability for fires in enclosures	New start	Years 3-5
6	Experimental and theoretical investigations of turbulent combustion	Fundamental	To develop an understanding of turbulent combustion sufficient to allow calculation of chemical source terms for simple flow configurations	Existing	Years 1-5
7	Vitiated burning in cone calorimeter	Fundamental	To investigate the effects of air vitiation on levels of CO produced in laminar burning	Existing	Years 1-2
8	Vitiated burning of buoyancy-driven turbulent flames	Both	To investigate the effects of air vitiation on turbulent flames, to test the global equivalence ratio concept for this type of burning	Existing	Years 1-2
9	Kinetic calculations for the investigation of upper-layer stability	Fundamental	To investigate the chemical stability of upper layers for appropriate ranges of gas concentrations and temperatures	New start	Years 1-3

#	RESEARCH COMPONENT	FUNDAMENTAL OR ENGINEERING	GOALS AND/OR PURPOSE	EXISTING RESEARCH OR NEW START	DURATION AND PROJECT TIMING
10	Experimental Investigation of the effects of heterogeneous chemistry on CO concentrations	Both	To characterize the effects of heterogeneous chemistry on soot particles on the stability of gas compositions in a heated upper layer	New start	Years 1-3
11	Burning behavior of upper-layer gases outside of small-scale enclosure	Engineering	To characterize conditions where burning of upper-layer gases occurs outside of enclosure fires and the effectiveness of such burning in removing CO	Existing	Years 2-4
12	Burning behavior of upper-layer gases outside of full-scale enclosure	Engineering	To characterize conditions where burning of upper-layer gases occurs outside of enclosure fires and the effectiveness of such burning in removing CO	New start	Years 3-4
13	Turbulence modeling of CO formation in enclosure fires	Both	Evaluate effectiveness of the laminar flamelet concept with k- turbulence modeling for predicting CO in enclosure fires	New start	Years 2-4
14	Development of data base for CO formation in full-scale fire tests	Engineering	To include appropriate reporting of CO measurements in large-scale fire test data base and access levels of CO which are observed	Existing	Years 1-2
15	Large-scale fire tests	Engineering	Perform accurate measurements of CO and other flame gases both within the enclosure and downstream for full-scale fires	Both	Years 1-5
16	Scaling studies	Engineering	Test effectiveness of scaling from small to full-scale tests, focus on the global equivalence ratio concept and correlations for burning of upper layer gases on exiting enclosure	New start	Years 3-5
17	Incorporation of CO formation in fire models	Engineering	Incorporate findings of CO priority project into CFR fire models	New start	Years 3-5
18	Project management	-	Effective project coordination	Existing	Years 1-5