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## Evaluation of a Near-Adiabatic Compression Process to Increase Fire Safety Within Oxygen Systems, Focusing on Non-Metals

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### ABSTRACT

One of the most important ignition mechanisms initiating burning in nonmetallic materials, which is directly linked to many large oxygen system fires, is the rapid or near-adiabatic compression of oxygen against a nonmetallic material. Adiabatic compression testing of components and systems is utilized worldwide to determine their compatibility in oxygen systems. However, limited research is available on how adiabatic compression energy is transferred to nonmetallic materials, leading to ignition. By characterizing the transfer of heat from hot compressed oxygen into the non-metal that occurs prior to ignition, an analytical model will be developed to describe this process. A transient model of non-metals in a pure oxygen environment is considered. The development of the mathematical model that simulates the behavior of non-metal ignition when subjected to a near-adiabatic compression process is presented. The ignition model investigates various physical mechanisms, such as heat transfer mechanisms, and reaction rates to determine processes involved during the transfer of heat from hot oxygen to a non-metal prior to ignition. The focus of

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this model is the gas/solid interface. This research is currently ongoing. Future work will validate the model experimentally before determining maximum safe compression rates to prevent the ignition of different classes of nonmetallic materials. The significance of this research is to increase the fire safety of oxygen systems by establishing a theoretical model to reduce, or eliminate, one of the most common mechanisms of ignition found within oxygen systems—that is, adiabatic compression.

### Keywords

adiabatic compression, fire safety, oxygen, non-metal, ignition, gas-phase reaction

## Introduction

Adiabatic compression is one of the most common mechanisms for the ignition of nonmetallic materials in an oxygen system. Nonmetallic materials and their composites are used in a wide variety of engineering applications. Non-metals, due to their relative ease of ignition as compared to metals, are often the primary source initiating oxygen system fires. Increasing oxygen pressure to improve system efficiency through operational and design changes increases the probability of material ignition, which results in an increase in fire occurrence. The theory of thermal ignition is based upon the basic concept that thermal energy input into a system is greater than thermal energy output [1]. The temperature rise by a near-adiabatic compression process is commonly calculated by assuming ideal gas behavior through the isentropic (reversible and adiabatic) relationship

$$T_f = T_i \left( \frac{P_f}{P_i} \right)^{k-1} \quad (1)$$

where:

$T_f$  = final temperature (abs);

$T_i$  = initial temperature (abs);

$P_f$  = final pressure (abs);

$P_i$  = initial pressure (abs);

$k$  = ratio of specific heats for oxygen (1.4).

As identified by multiple studies, the ideal gas assumption does not accurately calculate real gas behavior [2–4]. Newton et al. present a measurement technique for determining the temperature profile of oxygen in a typical pressure surge [5]. However, the temperature increase within the non-metal was not investigated. A transient ignition model for a nonmetallic polymeric reactive solid in contact with oxygen under external heating was investigated by Yuen et al. [6]. This model was developed for a generalized system and was not restricted to a particular ignition mechanism or system geometry. A heterogeneous reaction was assumed. Additionally, this model assumed ideal gas behavior and ignored convection motion in the gas phase, which was identified as a significant factor in the evaluation of oxygen-flow systems.

## Ignition Model 1

To understand the temperature profile of a non-metal solid over time, it was initially assumed that transient ignition was influenced only by heat transfer mechanisms. A schematic of the one-dimensional semi-infinite model used for analysis is shown in Fig. 1, where  $T$  is the temperature flow from the gas phase to the solid phase,  $q_{Conv}$  is convection into the solid, and  $q_{Cond}$  is the conduction through the solid. Ignition occurs when the surface temperature,  $T(0,t)$ , reaches the ignition temperature of the material. Surface emissivity is assumed to be one, with no heat generation within the test material, and the material is initially at an ambient surrounding temperature,  $T_i$ .

The energy equation for the solid phase can be written as

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha} \frac{\partial T}{\partial t}, \quad 0 < t, 0 < x < \infty \quad (2)$$

where:

$x$  = distance measured from the gas/solid interface;

$t$  = time;

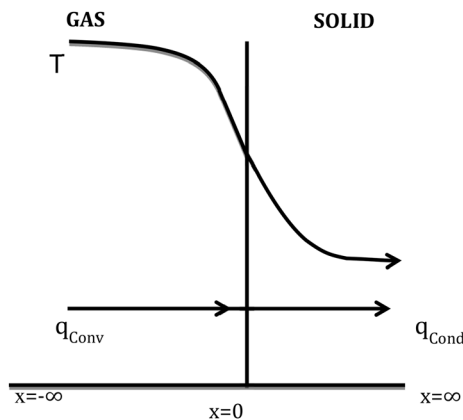
$\alpha$  = diffusivity of the solid.

Initial and boundary conditions are

$$\begin{aligned} T(x, 0) &= T_i \\ T(\infty, t) &= T_i \\ -kA \frac{\partial T(0, t)}{\partial x} &= h[T_\infty - T(0, t)] \end{aligned}$$

Using Laplace transforms to solve initial and boundary conditions [7], the solution of temperature for this model is

**FIG. 1** Schematic drawing of model geometry and coordinate system.



$$\frac{T(x,t) - T_i}{T_g - T_i} = \operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right) - \left[e^{\frac{hx}{k} + \frac{h^2 \alpha t}{k^2}}\right] \left[\operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}} + \frac{h\sqrt{\alpha t}}{k}\right)\right], \quad 0 < t, 0 < x < \infty \quad (3)$$

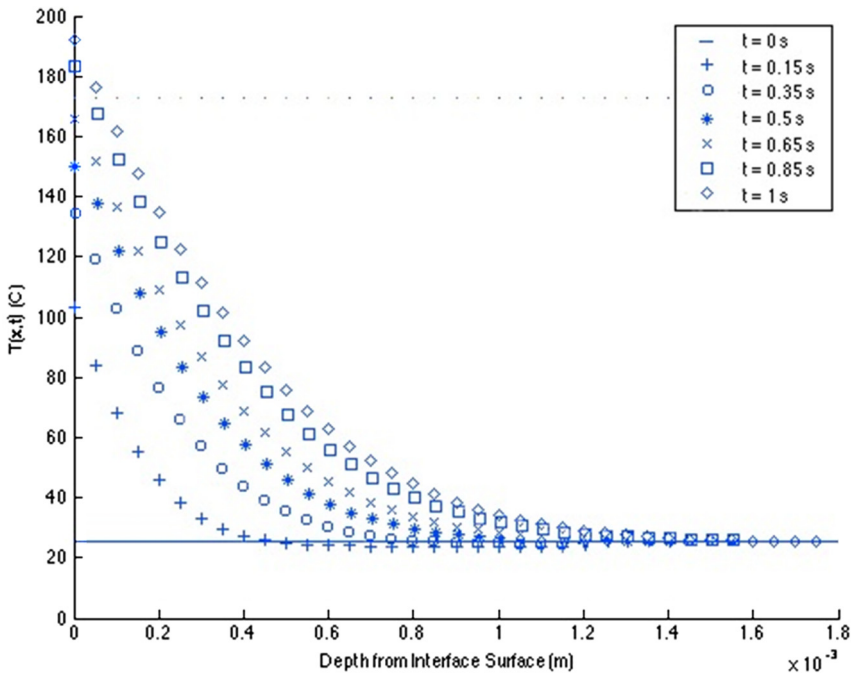
where:

- $\alpha$  = diffusivity of solid;
- $h$  = convection coefficient of gas;
- $k$  = conduction coefficient of solid.

The solution was modeled with the solid reagent as Buna-N (nitrile rubber), which has an autoignition temperature (AIT) of 173°C [8]. Results are illustrated in Fig. 2 using published thermophysical properties [8]. A straight line at  $T(x, t) = 173^\circ\text{C}$ , indicates the AIT temperature. Due to results from Newton [9], 500°C was selected as an appropriate approximation of gas temperature. A convection heat transfer coefficient of  $250 \text{ W m}^{-2}\text{K}^{-1}$  was utilized for this calculation [10]. With conductive heat transfer between the heated gaseous oxidizer and the less heated solid, the trend of temperature in the solid was expected.

Ignition by adiabatic compression has been observed to occur within 100 ms [9]. From Fig. 2, the rate of temperature rise is not adequate to represent ignition in a non-metal during an adiabatic compression process. This signifies ignition is not

**FIG. 2** Temperature in semi-infinite Buna-N as a function of depth and time for a convective boundary condition (in this case, temperature of the gas is 500°C).



determined solely by heat transfer mechanisms. A chemical reaction with Arrhenius dependence of the reaction rate on temperature can be utilized to include reaction intermediates.

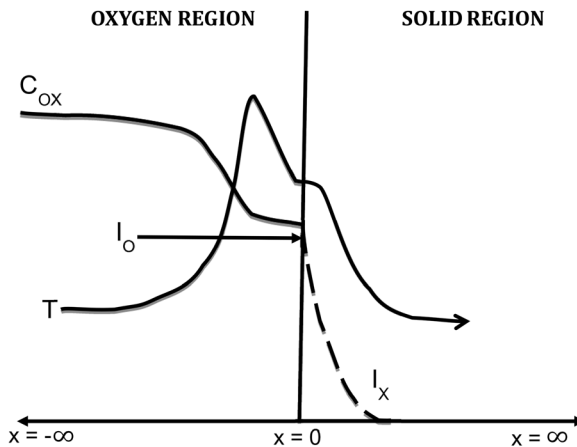
## Ignition Model 2

In the theory of ignition of a substance in the gaseous phase, external influence raises the surface temperature of the solid, such that it begins to degrade. The resulting pyrolysis products diffuse away from the surface and ignite with the surrounding gaseous oxidant by a second-order exothermal reaction [11]. Similar to many existing studies on gas-phase ignition of solid propellants [12–14], the mathematical formulation for this gas-phase ignition model is developed from a number of assumptions. The schematic diagram in Fig. 3 can represent the model of ignition in the gas phase, indicating the transfer of temperature ( $T$ ), oxygen concentration ( $C_{OX}$ ), and thermal emission ( $I_O$ ) from the gas phase to the solid phase.

Variation of temperature in the solid region is influenced by the pyrolysis of the material, the heating of the interfacial layer as a result of radiation absorption, and by the heat release as a result of photochemical degradation [15]. Pyrolysis of the material is assumed to be a one-step, zero-order gasification reaction. Eq 4 describes the governing equation for the variation of temperature over time in the solid region:

$$\frac{\partial T}{\partial t} = \alpha_s \frac{\partial^2 T}{\partial x^2} - h_s \frac{\partial T}{\partial x} - \pi \left( \frac{Q_{pyr} k_{0,s}}{c_s} \right) e^{-\frac{E_s}{RT}} + \left( \frac{1}{\rho_s c_s} \right) \frac{\partial I_x}{\partial x} + \frac{\mu Q_{pc} I_x}{\rho_s c_s}, \quad 0 < t, 0 < x < \infty \tag{4}$$

**FIG. 3** Schematic drawing of ignition model in a gaseous phase.



where:

- $\alpha_s$  = diffusivity of solid;
- $h_s$  = convective coefficient of solid;
- $Q_{pyr}$  = heat of pyrolysis reaction;
- $K_{0,s}$  = pre-exponential factor of solid;
- $c_s$  = concentration of solid;
- $E_s$  = activation energy of solid;
- $R$  = universal gas constant;
- $\mu$  = thermal emission absorption coefficient;
- $Q_{pc}$  = heat of photochemical degradation (in solid phase);
- $I_x$  = thermal emission absorption fraction;
- $\rho_s$  = density of solid;
- $c_s$  = specific heat of solid.

The variation of temperature in the gas region is influenced by heat release as a result of photochemical degradation [15]. Eq 5 describes the governing equation for the variation of temperature over time in the gaseous region:

$$\frac{\partial T}{\partial t} = \alpha_g \frac{\partial^2 T}{\partial x^2} - h_g \frac{\partial T}{\partial x} + \left( \frac{Qk_{0,g}}{\rho_g c_g} \right) c_{ox} c_f e^{-\frac{E_g}{RT}}, \quad 0 < t, -\infty < x < 0 \quad (5)$$

where:

- $\alpha_g$  = diffusivity of gas;
- $h_g$  = convective coefficient of gas;
- $Q$  = heat of photochemical degradation (in gas phase);
- $k_{0,g}$  = pre-exponential factor of gas;
- $c_{ox}$  = concentration of oxygen;
- $c_f$  = concentration of fuel (test sample);
- $E_g$  = activation energy of gas.

Eq 6 describes the governing equation for the variation of fuel concentration over time in the gas region. This equation considers the complete combustion of a gaseous fuel as a result of its reaction with the oxidant [15]:

$$\frac{\partial c_f}{\partial t} = D \frac{\partial^2 c_f}{\partial x^2} - h_g \frac{\partial c_{ox}}{\partial t} - k_{0,g} c_{ox} c_f e^{-\frac{E_g}{RT}}, \quad 0 < t, -\infty < x < 0 \quad (6)$$

where:

- $D$  = molecular diffusivity.

The following initial and boundary conditions will be applied to solve Eq 4, Eq 5, and Eq 6.

Initial conditions:

$$T(x, 0) = T_o$$

$$c_f(x, 0) = 0$$

Boundary conditions:

$$\begin{aligned}
 T(\pm\infty, t) &= T_o \\
 T_g(0, t) &= T_s(0, t) \\
 k_g \frac{\partial T(0, t)}{\partial x} &= k_s \frac{\partial T(0, t)}{\partial x} \\
 c_f(\infty, t) &= 0 \\
 \dot{m}_f &= c_f h_g - D \left( \frac{\partial c_f}{\partial t} \right)
 \end{aligned}$$

where:

$\dot{m}_f$  = mass fuel consumption.

The mass fuel consumption results from the in-depth pyrolysis. The objective is to solve the given system of equations for Model 2 for the temperature distribution as a function of depth and time with the given initial and boundary conditions. This work is currently ongoing.

## Conclusion and Future Work

This paper presents the development of a transient ignition model for a near-adiabatic compression process in a pure-oxygen system. It investigates various parameters required for an ignition to occur. The intended future work is to continue developing the model with reactive intermediates by developing a solution of temperature as a function of depth and time. Results will then be illustrated using a computer program, before comparison with Model 1, and experimental data. Once a model is established, an upper limit of the maximum “safe” compression rates can be determined based on an approximate solution to the governing equations.

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