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THERMODYNAMIC AND FLUID MECHANIC ANALYSIS OF RAPID PRESSURIZATION IN A DEAD-END TUBE

Final Report

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ABSTARACT

Three models have been applied to very rapid compression of oxygen in a dead-ended tube. Pressures as high as 41 MPa (6000 psi) leading to peak temperatures of 1400 K are predicted. These temperatures are well in excess of the autoignition temperature (750 K) of teflon, a frequently used material for lining hoses employed in oxygen service. These findings are in accord with experiments that have resulted in ignition and combustion of the teflon, leading to the combustion of the stainless steel braiding and catastrophic failure.

The system analyzed was representative of a capped off high-pressure oxygen line, which could be part of a larger system. Pressurization of the larger system would lead to compression in the dead-end line, and possible ignition of the teflon liner. The model consists of a large plenum containing oxygen at the desired pressure (500 to 6000 psi). The plenum is connected via a fast acting valve to a stainlees steel tube 2 cm inside diameter. Opening times are on the order of 15 ms. Downstream of the valve is an orifice sized to increase filling times to around 100 ms. The total length from the valve to the dead-end is 150 cm. The distance from the valve to the orifice is 95 cm.

The models describe the fluid mechanics and thermodynamics of the flow, and do not include any combustion phenomena. A purely thermodynamic model assumes filling to be complete upstream of the orifice before any gas passes through the orifice. This simplification is reasonable based on experiment and computer modeling. Results show that peak temperatures as high as 4800 K can result from recompression of the gas after expanding through the orifice.

An approximate transient model without an orifice was developed assuming an isentropic compression process. An analytical solution was obtained. Results indicated that fill times can be considerably shorter than valve opening times. Thus, even though manually opening a valve is slow compared to a fast acting valve, fill times can still be short. For a 100 cm long tube with a valve opening time of 100 ms, the fill time is about 30 ms.

The third model was a finite difference, 1-D transient compressible flow model. The code was obtained from Sandia Livermore and applied to the system. Results from the code show the recompression effect but predict much lower peak temperatures than the thermodynamic model. The difference is due mostly to the complete lack of mixing in the thermodynamic model. Pressure oscillations upstream of the orifice are predicted by this model as observed experimentally; however, damping is greater in the computer model.

INTRODUCTION

Considerable effort has been made at the White Sands Test Facility (WSTF) to characterize and understand the phenomena associated with the rapid pressurization of flex hoses containing pure oxygen. Pressures in excess of $6000\,psig$, with pressurization rates as high as $600,000\,psi/s$ have been utilized. The primary concern involves the possibility of combustion. This can result from the high temperatures generated from the compression of the low pressure oxygen originally in the system, when exposed to a high pressure source. Valve opening times must be short ($\approx 0.1\,s$), but test have shown that opening times of this duration are within the ability of a person to achieve manually.

At present the mechanisms that lead to hose failure are believed to be pyrolysis of a portion of the teflon lining, followed by ignition of these pyrolysis products, followed in some cases by the ignition of the stainless steel braiding. Even in those cases which do not result in catastrophic failure, the teflon monomer and partially reacted species such as carbonyl fluoride (COF_2) have been observed. The later compound is highly toxic and could pose a serious health risk if the flex hose were part of a life support system.

To date, most of the effort at WSTF has been directed toward whether or not hoses met certain criteria regarding acceptable failure rates. However, in addition to these efforts a program [1] aimed at a more basic understanding of the phenomena of compression initiated combustion has been underway for about two years. These efforts have been primarily experimental in nature, and have provided the results mentioned above regarding the sequence of events that can lead to catastrophic failure. Current experimental efforts are directed to *in-situ* spectroscopic methods for measuring pressure and temperature in real time. These data will not only be valuable in themselves, but will provide input to, and verification of, flow models developed. The bulk of this report is concerned with various models, of varying degrees of complexity, for describing the compression process.

At the start of this summer program, modeling of the compression process itself had been based on a very simple picture of the system. Estimation of the maximum temperature near the dead end (assumed worst case) of a hose or tube was determined from the isentropic ideal gas relation between pressure and temperature. This relation is shown in Eq. 1.

$$\left(\frac{T_2}{T_1}\right) = \left(\frac{P_2}{P_1}\right)^{\frac{\gamma-1}{\gamma}} \tag{1}$$

Here γ is the ratio of specific heats, assumed to be constant with respect to temperature.

The model assumes piston like compression of the low pressure gas by the high pressure gas. For a gas initially at ambient conditions and then pressurized to $6000\,psig$ a final temperature of 1370°C is theoretically possible. The limitations of this model are readily admitted. The assumed isentropy precludes friction, heat transfer, and mixing. A more realistic model could have great utility in providing predictions for configurations that cannot be conveniently obtained via experimentation, and in addition as a starting point for a model that includes combustion phenomena.

In the sections that follow several models are presented based on various assumptions. The order of presentation is essentially from the simplest to the most complex. A final section will give recommendations for further model development. It should be kept in mind that a flow model, no matter how sophisticated, will be incomplete without the chemistry of pyrolysis and combustion included. However, the phenomena involved are quite complicated in detail, and an initial effort that treats the flow as decoupled from the combustion is considered worthwhile and prudent.

REAL GAS EFFECTS

The simplest improvement on the isentropic ideal gas model is to include real gas behavior. To assess the importance of real gas effects reference is made to a generalized compressibility chart. The critical temperature and pressure of oxygen are $158.4\,K$ and $5.08\,MPa$ respectively. Based on the ideal gas relation, compression from ambient to $6000\,psig$ ($\sim 41\,MPa$) will result in a gas temperature of 1370°C. The reduced temperature and pressure are 10.4 and 8.03 respectively. The compressibility factor Z is 1.08. This value suggests that that real gas effects should not be significant. However, the temperature effect on specific heats may still be important.

To determine the actual relation between temperature and pressure during isentropic compression a computer program was written. The real-gas model used was *van der Waals'* with constants 'a' and 'b' calculated using the critical point method. The expression to determine T versus P is given in Eq. 2.

$$\left(\frac{\partial T}{\partial P}\right)_s = \frac{T}{c_p}\left(\frac{\partial v}{\partial T}\right)_p \tag{2}$$

The results of the integration are shown in Fig. 1. Also shown in this figure is the curve based on Eq. 1. and a curve allowing for variation in specific heat with temperature, but assuming ideal gas behavior. This last relation was calculated from the expression

$$P = P_o\, exp\left[\frac{1}{R}\int_{T_o}^{T}\frac{c_p(T)}{T}dT\right] \tag{3}$$

where P_o and T_o are initial values, such as ambient conditions, and $c_p(T)$ is the constant pressure specific heat. The functional form of $c_p(T)$ was taken from reference [2].

Inspection of Fig. 1 reveals two important features. The first is that compressibility effects are not significant as anticipated. The second feature is that the temperature dependence of $c_p(T)$ is fairly important. For example, if ambient O_2 is compressed isentropically to $5000\,psig$, ($34.5\,MPa$) applying Eq. 1 predicts a temperature of 1295°C. If variable specific heat is accounted for this temperature drops to 1066°C. If both real gas behavior and variable specific heats are considered the predicted temperature is 1092°C. Each of the curves forms a straight or nearly straight line on a log-log plot. Thus, the two variable-property curves can be fit to functions of the form of Eq. 1. A least-squares method was used to find the appropriate exponent n in Eq. 4.

$$\left(\frac{T}{T_o}\right) = \left(\frac{P}{P_o}\right)^n \tag{4}$$

The three values for n and the correlation coefficient r^2 are listed below.

ideal gas with constant specific heats ($\gamma = 1.395$)
$n = 0.2829$ $\quad$ $r^2 = 1.0000$

ideal gas with variable specific heats
$n = 0.2599$ $\quad$ $r^2 = 0.9987$

real gas (*van der Waals*) with variable specific heats
$n = 0.2632$ $\quad$ $r^2 = 0.9989$

The values on n for the last two cases strickly apply to $T_o = 300\,K$ and $P_o = 100\,kPa$; however, small deviations from these values should cause little error.

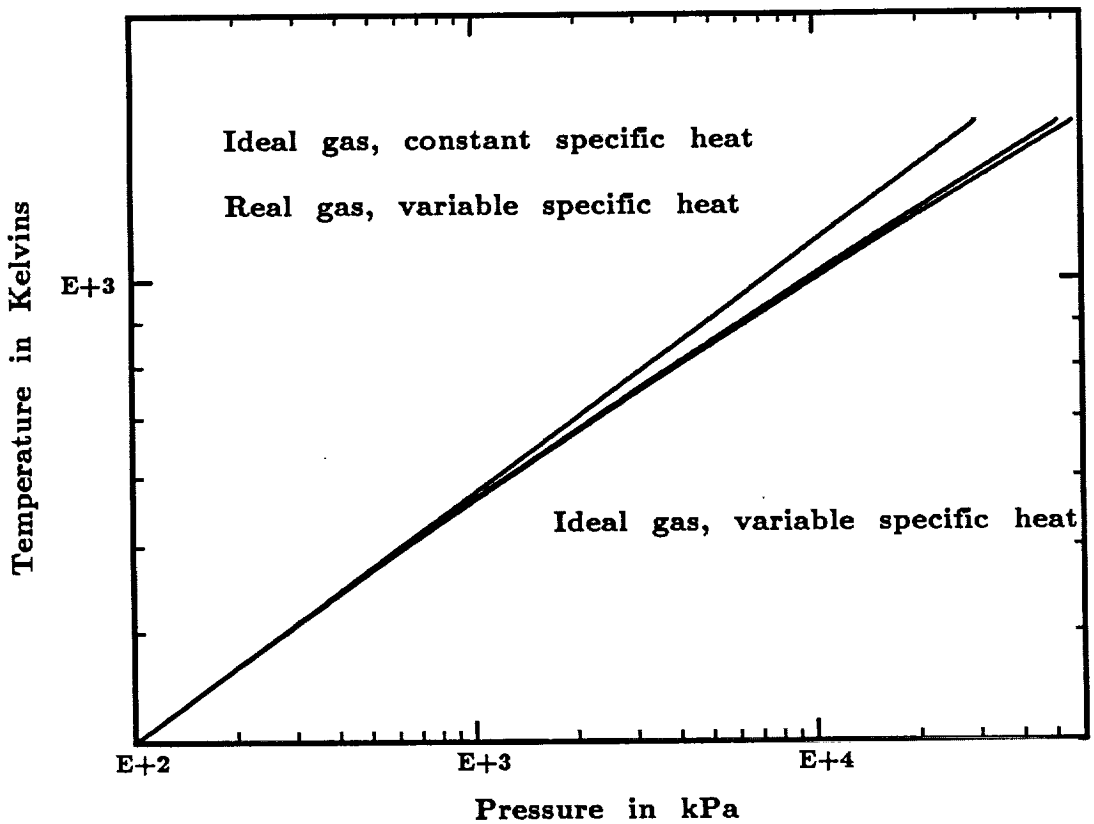

Figure 1.- Isentropic temperature-pressure relations.

SIMPLE THERMODYNAMIC MODELS

Most of the experiments conducted at WSTF involving rapid pressurization of flex hoses or hard lines involve an orifice. The purpose of the orifice is to decrease the pressurization rate from those attainable by the fast acting valve. Valve opening times between 13 and 18 *ms* are typical; pressurization times would be of the same order. The orifice was sized so that pressurization times were on the order of 100 *ms*.

As a first approximation the orifice was accounted for in the following manner. The valve is assumed to open instantly, and high pressure plenum gas pressurizes the gas in the volume upstream of the orifice before any significant flow occurs through the orifice. Next, gas flows through the orifice with the pressure dropping to the local downstream pressure. Eventually the pressure is everywhere uniform and equal to the plenum pressure (assumed constant due to large volume). Additional assumptions include: ideal gas behavior, constant specific heats, no heat transfer, and no frictional losses. Pressure is assumed to be spatially uniform on each side of the orifice.

Even with all these assumptions and the simple nature of the model, several cases need to be considered. Two broad classes result from assuming piston like compression of the gas downstream of the orifice on the one hand, and complete mixing on the other. In both cases the gas originally upstream of the orifice is assumed to be compressed in a piston like manner. Two subcases result depending on whether or not the initially compressed gas is of sufficient quantity to compress the gas downstream of the orifice without any driver gas (gas originally in the plenum) passing through the orifice. The results are presented below for these cases.

Nomenclature:

A subscript refers to gas originally between valve and orifice

B subscript refers to gas originally downstream of orifice

nm subscript refers to no mixing

cm subscript designates complete mixing

i initial conditions

f final conditions

P_f final pressure equal to plenum pressure

P_i initial pressure (same for gases A and B)

$\Re$ pressure ratio $P_f/P_i \geq 1$

γ ratio of specific heats

ϑ_{A_i} volume between valve and orifice

ϑ_{B_i} volume downstream of orifice

T_s isentropic temperature based on Eq. 1

The formulae for the various cases are presented based on whether or not driver gas passes through the orifice. With the various assumptions borne in mind, the limiting case for no flow through the orifice is determined from Eq. 5.

$$\left.\frac{\vartheta_{A_i}}{\vartheta_{B_i}}\right)_{critical} = \frac{\Re - 1}{\gamma \Re^{\frac{\gamma-1}{\gamma}}} \tag{5}$$

This result applies to both mixing and nonmixing of gases A and B.

No Driver Gas Through Orifice And No Mixing

$$\left.\frac{T_B}{T_i}\right)_{nm} = \frac{T_s}{T_i} = \Re^{\frac{\gamma-1}{\gamma}} \qquad \text{Gas B} \tag{6}$$

$$\left.\frac{T_A}{T_s}\right)_{nm} = \frac{\gamma(\Re - \Re^{\frac{\gamma-1}{\gamma}})}{\Re - 1} \qquad \text{Gas A} \tag{7}$$

The volume of Gas B after compression can be found from Eq. 8.

$$\frac{\vartheta_{B_f}}{\vartheta_{B_i}} = \Re^{-1/\gamma} \tag{8}$$

Complete mixing downstream of orifice

$$\frac{T_{cm}}{T_s} = \frac{\gamma \Re}{\gamma \Re^{\frac{\gamma-1}{\gamma}} + \Re - 1} \tag{9}$$

Some Driver Gas Through Orifice And No Mixing

Before any Gas A passes through the orifice it is compressed to P_f. This state is referred to as state 1.

$$\frac{T_{A_1}}{T_i} = \Re^{\frac{\gamma-1}{\gamma}} \tag{10}$$

Due to the nature of the derivation a second intermediate state (state 2) is determined. This state occurs when all of Gas A has just passed through the orifice. Note that the temperatures are normalized to T_s rather than T_i.

$$\left[1 + \frac{\vartheta_{A_i}}{\vartheta_{B_i}} \Re^{\frac{\gamma-1}{\gamma}} \left(\gamma - \frac{T_{A_2}}{T_s}\right)\right]^{\frac{1}{\gamma-1}} = 1 + \frac{\vartheta_{A_i}/\vartheta_{B_i}}{\Re^{\frac{1-\gamma}{\gamma}} \frac{T_s}{T_{A_2}} + \frac{\vartheta_{A_i}}{\vartheta_{B_i}} \left(\gamma \frac{T_s}{T_{A_2}} - 1\right)} \tag{11}$$

$$\frac{T_{B_2}}{T_s} = \Re^{\frac{1-\gamma}{\gamma}} + \frac{\vartheta_{A_i}}{\vartheta_{B_i}} \left(\gamma - \frac{T_{A_2}}{T_s}\right) \tag{12}$$

$$\frac{P_2}{P_i} = \Re \left(\frac{T_{B_2}}{T_s}\right)^{\frac{\gamma}{\gamma-1}} \tag{13}$$

The final state (state 3) is given by:

$$\frac{T_{A_3}}{T_s} = \frac{1}{\Re^{\frac{1-\gamma}{\gamma}} \frac{T_s}{T_{A_2}} - \frac{\vartheta_{A_i}}{\vartheta_{B_i}} \left(1 - \gamma \frac{T_s}{T_{A_2}}\right)} \tag{14}$$

$$\left.\frac{T_{B_3}}{T_s}\right) = 1 \tag{15}$$

The driver gas temperature is assumed to remain constant at T_i, except for that portion that passes through the orifice. The temperature of this portion is given by:

$$\frac{T_{D_3}}{T_i} = \frac{\gamma}{1 + \frac{\left(\frac{\vartheta_{A_i}}{\vartheta_{B_i}} \frac{T_{A_2}}{T_s} + \frac{T_{B_2}}{T_s}\right)\left(\frac{T_s}{T_{B_2}} - 1\right)}{\Re^{1/\gamma} - \frac{\vartheta_{A_i}}{\vartheta_{B_i}} \frac{T_{A_3}}{T_s} - \frac{T_{B_2}}{T_s}}} \tag{16}$$

In order to determine T_{A_3} and T_{D_3} (also T_{B_2} and P_2) the values of $\vartheta_{A_i}/\vartheta_{B_i}$, $\Re$, and γ must be known. With these values Eq. 11 is solved iteratively for $T_{A_2}/T_s)_{nm}$ and substituted into Eqs. 14 and 16.

Complete mixing

$$\left.\frac{T_3}{T_i}\right)_{cm} = \frac{\Re}{\frac{1}{\gamma}(\Re - 1) - \left(\frac{\vartheta_{A_i}}{\vartheta_{B_i}}\right)\left(\Re^{\frac{\gamma-1}{\gamma}} - 1\right) + 1} \tag{17}$$

Results for no driver gas through the orifice and no mixing were determined for the values are listed below.

$$T_i = 300\,K \qquad \Re = 300 \;\; (\sim 4400\,psig) \qquad \gamma = 1.395 \;\; (O_2 \text{ value})$$

The final temperature of Gas B is $1508\,K$ as is the temperature of Gas A when first compressed upstream of the orifice. However, the final temperature of Gas A that passes through the orifice is $2076\,K$ showing the recompression effect.

TRANSIENT ISENTROPIC MODEL

An approximate model was developed for the filling of a tube or hose with only a valve in the system, no orifice was included. The model is applicable to moderate rates of filling such that $\frac{\partial P}{\partial x}$ is negligable. This condition will be satisfied when $t_f \ll t_a$. Here t_f is the characteristic time to fill the hose, and t_a is the wave relaxation time. The wave relaxation time is given by Faeth [3] as L/a, where L is the length of the tube and a is the velocity of sound. For a $1\,m$ tube and $a = 350\,m/s$, $t_a = 2.8\,ms$. From a practical standpoint the filling time should be considerably greater than twice this value. Thus t_f should be at least $60\,ms$. For the fast acting valve this condition is not met. However, manual valve opening times are at least this long.

The model was further simplified by assuming the following:

1. isentropic compression downstream of valve
2. no axial mixing or diffusion
3. no heat transfer to tube wall
4. no chemical reactions
5. ideal gas model with constant specific heats
6. temperature of gas passing through valve is taken as T_D (plenum temperature)

To obtain the results desired the conservation equations for energy and mass must be solved simultaneously. The momentum equation need not be solved because of the assumption of no spatial variation in pressure. In addition to the two conservation equations, the equation of state and the isentropic relation between temperature and pressure are employed. The appropriate equations are provided in Eqs. 18 through 21.

Energy
$$c_v \frac{\partial \rho T}{\partial t} = -c_p \frac{\partial \rho T V}{\partial x} \tag{18}$$

Mass
$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho V}{\partial x} \tag{19}$$

Equation of State
$$P = \rho R T \tag{20}$$

Process
$$\frac{DT}{Dt} = \frac{\gamma - 1}{\gamma} T_i \, P(\tau)^{\frac{1-\gamma}{\gamma}} \frac{1}{P^{\gamma}} \frac{DP}{Dt} \tag{21}$$

Equation 21, labeled as process, is the isentropic relation between pressure and temperature. The pressure designated $P(\tau)$ is the pressure at $t = \tau$, which is the time when the fluid element passed through the orifice. It is Eq. 21 which is used to determine temperature from pressure.

The solution is comprised of two time domains. The first is characterized by choked flow at the orifice. The second domain involves unchoked flow. The transition from one regime to the other may or may not occur while the valve is still opening. The most rapid pressure rise occurs when choked flow is present and the valve is fully open. This is so since the rate of pressure increase is directly proportional to the flow area of the valve. Formulae for mass flux and pressure rise rate were taken directly from Faeth [3]. Here the solution for $P(t)$ is given for a valve area that increases linearly with time.

$$A_v(t) = A_m \frac{t}{t_o} \tag{22}$$

Here A_m is the maximum area of the valve and t_o is the time to open. Note that A_m is alway less than or equal to the area of the tube. The initial condition is $P = P_i$ and $T = T_D$ at $t = 0$. Thus, for choked flow and $t \leq t_o$

$$\frac{P}{P_D} = \frac{P_i}{P_D} + \frac{\gamma\, B\, a_D\, A_m}{2\vartheta_{tube}} \frac{t^2}{t_o} \tag{23}$$

where a_D is the sound speed at T_D, and B is a function of γ with a value near unity.

The condition for choking is

$$\frac{P}{P_D} \leq \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} \tag{24}$$

Substitution of Eq. 24 into Eq. 23 permits the unchoking time t_{uc} to be calculated, provide $t_{uc} \leq t_o$, the most likely case.

$$t_{uc} = \sqrt{\left[\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} - \frac{P_i}{P_D}\right] \frac{2\vartheta_{tube}}{\gamma\, B\, a_D\, A_m} t_o} \tag{25}$$

The limiting case where $t_{uc} = t_o$ occurs when

$$t_o = t_o^* = \left[\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} - \frac{P_i}{P_D}\right] \frac{2\vartheta_{tube}}{\gamma\, B\, a_D\, A_m} \tag{26}$$

Thus the unchoking time for $t_{uc} \leq t_o$ becomes

$$t_{uc} = \sqrt{t_o^*\, t_o} \tag{27}$$

For the purpose of an example air is chosen at ambient conditions. In addition, let $A_m = A_{tube}$ and the length of the tube be $1\,m$. For a pressure ratio $\Re = 10$, $t_o^* = 0.0030\,s$. For $\Re = 100$, $t_o^* = 0.0037\,s$. Inspection of Eq. 26 shows that as $\Re \to \infty$, $t_o^* \to 0.0038\,s$. These times are so short that it will almost alway be the case that unchoking will occur before the valve is fully open. For $t_{uc} < t < t_o$

$$\frac{P}{P_D} = \left\{1 - \left[\left(\frac{\gamma-1}{\gamma+1}\right)^{\frac{1}{2}} - \frac{\gamma-1}{\gamma}\frac{C}{4}\left(t^2 - t_{uc}^2\right)\right]^2\right\}^{\frac{\gamma}{\gamma-1}} \tag{28}$$

where the constant C is given by

$$C = \frac{\gamma\, a_D\, A_m / t_o}{\vartheta} \left(\frac{2}{\gamma-1}\right)^{\frac{1}{2}}$$

For $t > t_o > t_{uc}$ the appropriate equation is

$$\frac{P}{P_D} = \left\{1 - \left[\left(1 - \left[\frac{P_o}{P_D}\right]^{\frac{\gamma-1}{\gamma}}\right)^{\frac{1}{2}} - \frac{\gamma-1}{\gamma}\frac{C}{2}(t - t_o)\right]^2\right\}^{\frac{\gamma}{\gamma-1}} \tag{29}$$

where P_o/P_D is determined from Eq. 28 when $t = t_o$. Pressure versus time for the case described above with $\Re = 100$ and $t_o = 100\,ms$ is plotted in Fig. 2. The time for unchoking is $19.2\,ms$. It is interesting to note that the time to fill the tube is $30\,ms$, considerably less than the $100\,ms$ valve opening time.

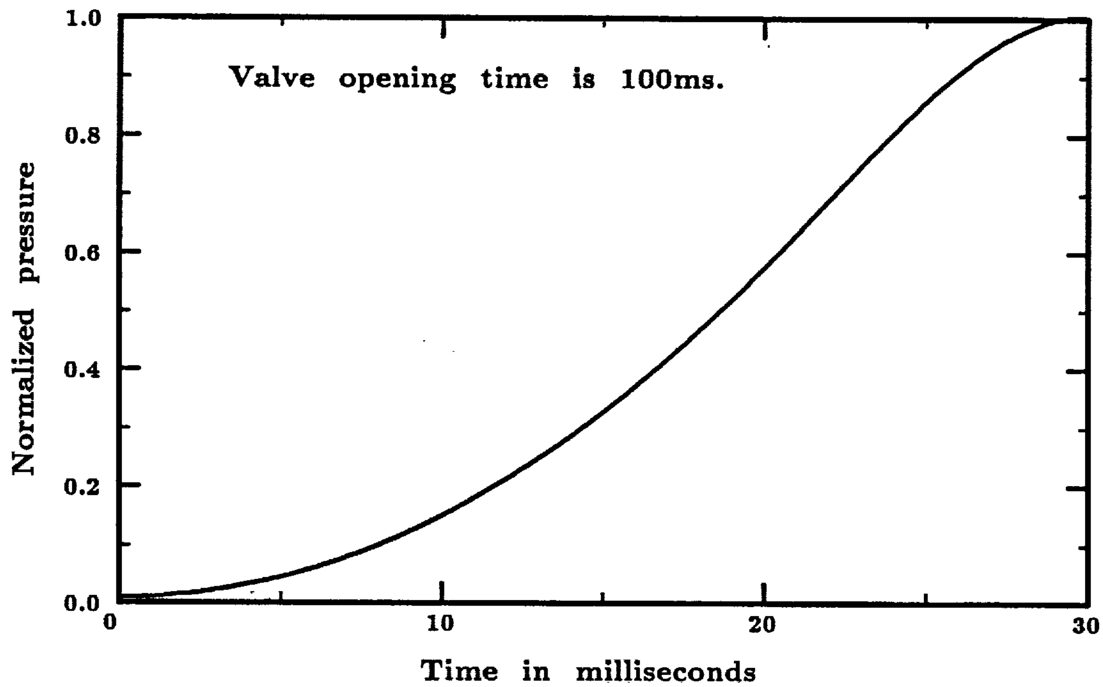

Figure 2.- Pressure rise from isentropic model

COMPUTER RESULTS USING TOPAZ

In the words of the author of the computer code "TOPAZ is a *user friendly* computer code for modeling the one-dimensional-transient physics of multi species gas transfer in arbitrary arrangements of pipes, valves, vessels, and flow branches". The author is W. S. Winters of the Computational Mechanics Division, Sandia National Laboratories, Livermore, CA. Dr. Winters was most helpful and cooperative in making the source code available to me. For documentation on TOPAZ see [4,5,6,7].

Some experimental results for pressure were available at the start of this computational work. The exact physical setup appropriate for the data was not known, but data both upstream of the orifice and at the dead-end were available. Therefore, the general characteristics of the pressure transients were known. These characteristics included a very rapid and oscillatory pressure rise upstream of the orifice, and a much slower and well behaved pressure rise at the dead-end. The oscillations are believed to be due pressure waves traversing the distance between the high pressure plenum and the orifice. These oscillations were observed in the computed results as well.

The system modeled in TOPAZ was a $1\,m^3$ spherical high pressure plenum. Gas from the plenum flowed through five identical valves in parallel. Each valve when fully open is one-fifth the area of the main pipe. The first part of the main pipe was $95\,cm$ long and $2\,cm$ inside diameter. This pipe fed into an orifice $1\,cm$ long and $3\,mm$ in diameter. The orifice was followed by another $2\,cm$ diameter pipe $48\,cm$ long. Heat transfer was accounted for via the 'constant wall temperature' model.

Results are shown in Figs. 3 and 4. Figure 3 shows three pressure traces. Examination of the dead-end trace shows that the fill time is $\sim 90ms$. This fill time is somewhat less than the experimental results indicating that the orifice should be a little smaller. The other two traces are for locations just upstream of the orifice. The pressurization rates are much higher than at the dead-end, and show that the approximation (no gas passing through orifice while upstream is pressurized) made in the thermodynamic analysis section was reasonable.

The control element (CE (control volume)) just upstream of the orifice experiences considerable pressure overshoot (factor of 1.8). The exact amount of the overshoot depends on how the system is modeled. Details such as the CE length both before and in the orifice can change the maximum value. However, the frequency of the oscillations and the time to decay to the final pressure are not significantly effected. This extreme overshoot only occurs in the CE just before the orifice independent of other changes. Further study is required to determine if this overshoot is real, or a manifistation of the numerical model.

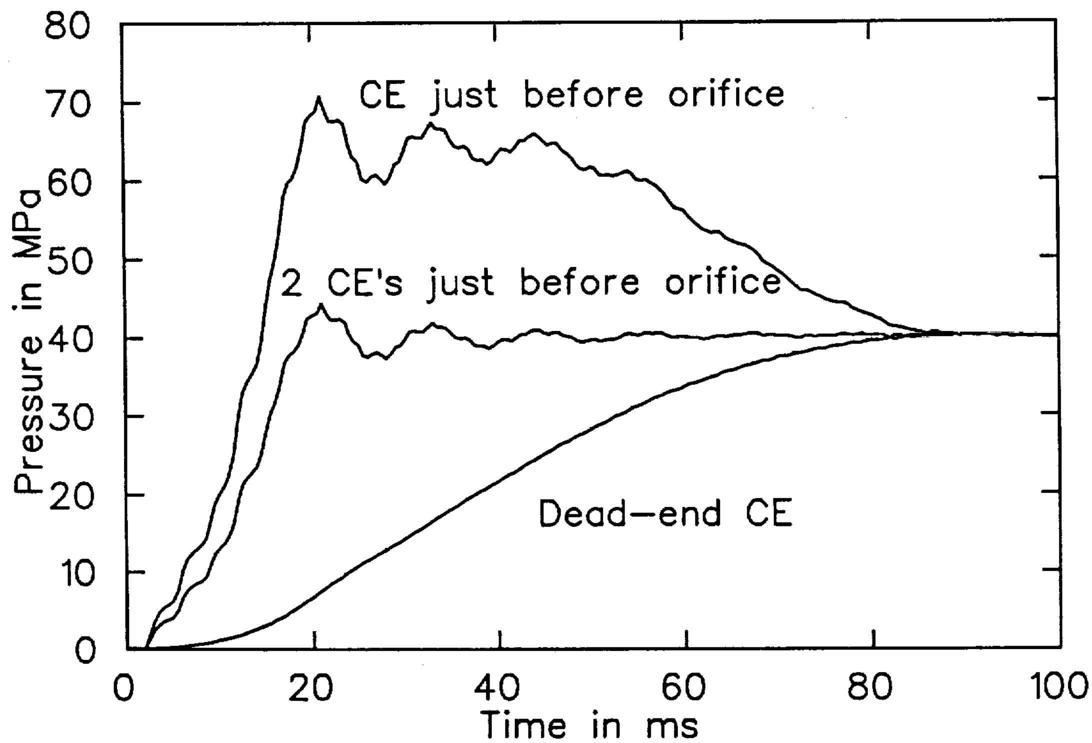

Figure 3.- Pressure rise in tube with 3 *mm* orifice. Upper curves are just upstream of orifice, lower curve is at very end of tube.

Temperature traces at and near the dead-end are shown in Fig. 4. If the order of the curves at 100 *ms* is examined, the highest temperature occurs at the dead-end with temperatures decreasing as one moves upstream. At least two significant features need to mentioned. The first feature is that the presence of the orifice results in a higher maximum temperatures. For a straight tube with no orifice, a maximum temperature of $\sim 980\,K$ was reached. With an orifice a maximum temperature near $1400\,K$ was reached. Thus, the recompression effect predicted earlier using thermodynamics only is confirmed; however, the effect is much smaller. The second feature is that the region that experience temperatures in excess of $750\,K$ (autoignition temperature of PTFE) is much larger than for a straight tube.

The placement of the orifice is important. If the orifice is located close to valve very little gas is initially pressurized and very little high temperature gas is recompressed. This means that pressurization rates can be controlled via an orifice with little unwanted recompression effects. On the other hand, a system in the field may contain restrictions some distance from the high pressure source and the dead-end and not be properly modeled unless the orifice is placed at the appropriate distance from the source.

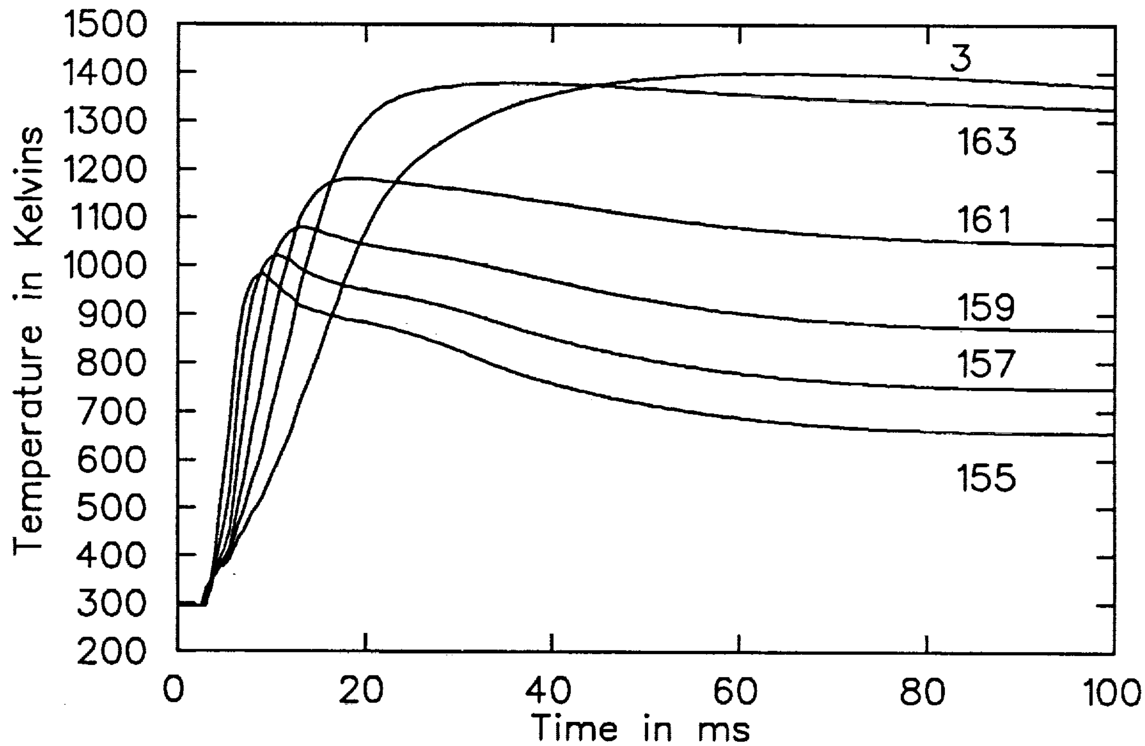

Figure 4.- Pressure rise in tube with 3 *mm* orifice. Distance is referenced from dead-end, curve 3 (0-3cm), curve 163 (3-8cm), curve 161 (8-13cm), curve 159 (13-18cm), curve 157 (18-23cm), curve 155 (23-28cm).

EXPERIMENTAL RESULTS

The available experimental results apply to a system somewhat different in detail to the system modeled by **TOPAZ**. The data are useful since they are "real" and because they show that **TOPAZ** is able to model the main features. The pressure data is considered most reliable because the response of the piezoelectric transducers is more than sufficient to capture any of the observed transients. The temperature data was obtained with a thin film thermocouple mounted at the dead-end. Only a very small portion of the tip was exposed and may have been within a thermal boundary layer after a very short time. There is also some question as to what the transient response characteristics are for the thin film thermocouple. A fairly sophisticated heat transfer analysis would be required to determine the *in situ* behavior.

Pressure traces are shown in Figs. 5 and 6 which were taken prior to the Summer of 1989. Mr. Dwight Janoff (now at JSC) made these data available, additional results are available. None of the traces was converted to pressure; however the reservoir pressure was 6000 *psig*. The relation between the vertical scale (mV) and pressure is fairly linear at early times. The apparent decrease in pressure observed beyond 0.2 *s* is not real and is due to behavior of the piezoelectric transducer. Figure 5 shows the pressure rise at the dead-end. Fill times are about 150 *ms*. Figure 6 shows the pressure history just before the orifice. Note that the rise to peak pressure is very rapid ($\sim$ 20 *ms*). The oscillations are considered real and not due to the transducer. The **TOPAZ** results also show oscillations, but not as persistent as in the actual data. In both the experimental results and the computer predictions, the upstream pressure transients continue until the downstream pressure has reached its final value. The other significant difference between the data and the predictions is the degree of overshoot. The data indicates a factor of 1.3, versus 1.8 from **TOPAZ**.

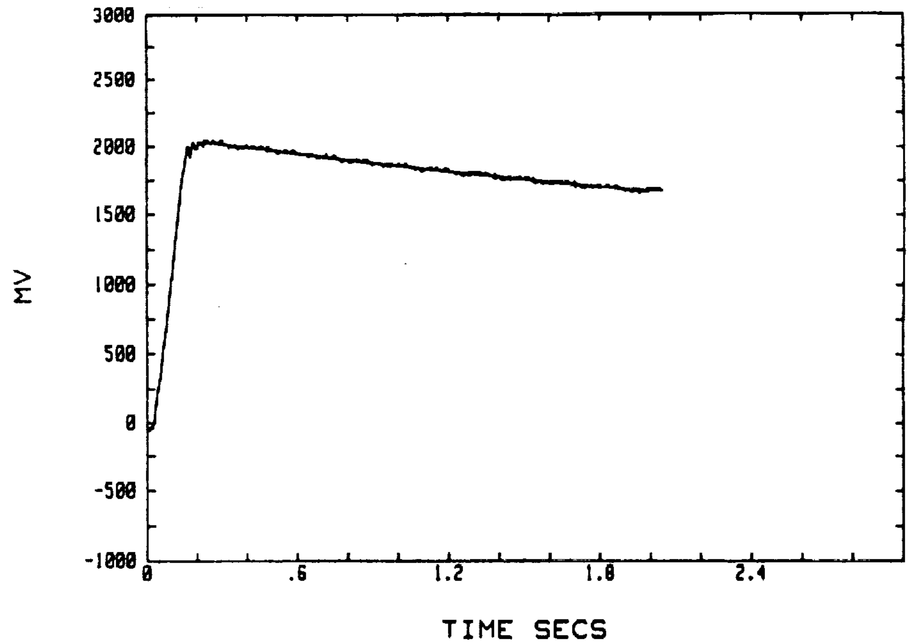

Figure 5.- Pressure trace at dead-end, orifice in place. Peak pressure was ~ 6000 *psi*.

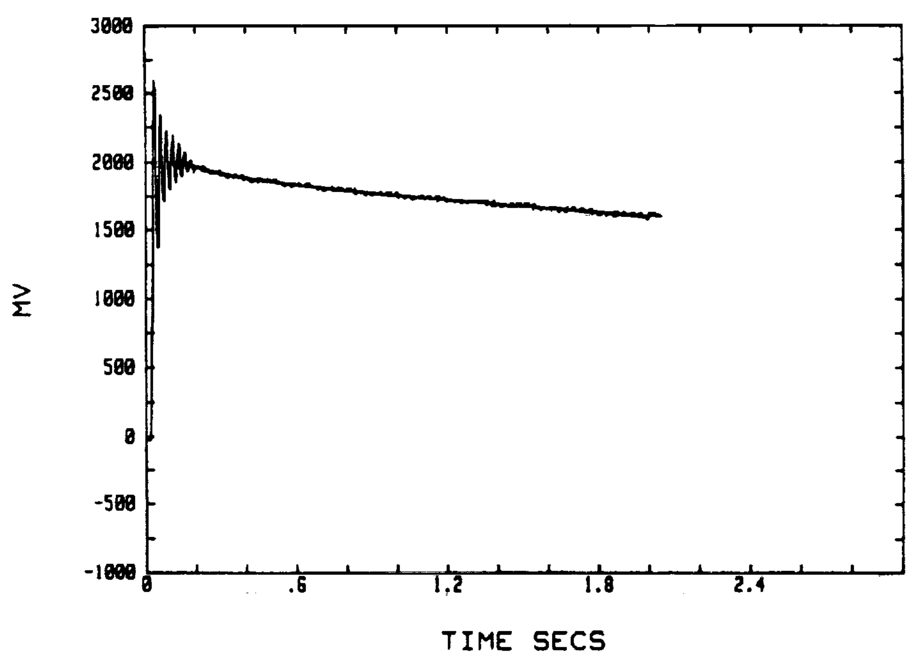

Figure 6.- Pressure trace just upsteram of orifice. Peak pressure was ~ 6000 *psi*.

CONCLUSIONS

The highly transient nature of the rapid compression process requires that the compressible form of the Navier-Stokes equation be solved. At present the 1-D form of these equations provides useful results, although further assessment is required to determine what the limitations are. These limitations could include frictional modeling, heat transfer modeling, and valve modeling. Results based on the purely thermodynamic model are valuable to illustrate the effects of recompression and mixing versus non-mixing models, but are not quantitatively accurate. The approximate 1-D isentropic model is restricted to slow filling rates and no orifice, but allows very quick results to be obtained. In addition, this approximate model being in an analytical form allows the dependence of fill time on various parameters to be easily determined. One result from this model is that filling times are only partially dependent on valve opening times. In general the fill time is much less than the valve opening time if the opening is performed manually.

The computer results from the code **TOPAZ** reproduce the experimental results reasonably well. Some of the differences are due to the actual experimental system not being modeled exactly in the code. The dominant feature that shows up both experimentally and theoretically is damped pressure oscillations upstream of the orifice. The code also predicts a recompression effect due to the presence of an orifice. The net results of this are higher peak temperatures and a larger region above the autoignition temperature of teflon. Thus, if an actual oxygen system has an orifice (or a partially opened valve) in the piping, higher peak temperatures can be obtained than would be expected. In either case the peak temperatures are calculated to be less than temperatures based on adiabatic compression, although only somewhat less with the recompression effect accounted for.

TOPAZ results suggest that heat transfer is not a significant factor during the first 150 *ms* or so. These times are thought to be sufficiently long to allow ignition to take place. The major increase in temperature takes place at very early times. This is due to the dependence of temperature on pressure . The adiabatic model of Eq. 1 shows that temperature rises most rapidly at the low pressures. Thus, high temperatures can be reached in just a few 10's of millseconds.

RECOMMENDATIONS

Several questions remain to be answered regarding the heating phase of the rapid compression (before significant pyrolysing or combustion). These questions are:

1. How do the various parameters of the problem effect final temperature?
2. Is the valve model used in **TOPAZ** 'good enough'?
3. What are the actual temperatures in the system?
4. Does the temperature drop very sharply right at the dead-end?
5. Is axial mixing significant?

To answer these questions the following recommendations are suggested:

1. continue calculations using **TOPAZ** to finish the parametric study of the problem,
2. apply existing 2-D codes to the problem to assess the accurateness of the 1-D code,
3. build an experimental system that is as simple as possible so that code predictions can be unambiguosly compared (all dimesions and parameters of the system must be known),
4. instrument the system for both pressure and temperature (either a 'hot-wire' method or optical technique needs to be used for temperature),
5. perform tests with nitrogen compressed by oxygen to assess mixing effects.

All code predictions require extensive amounts of CPU time. The VAX 8530 requires up to 65 hours to complete some runs. A 2-D code is expected to run longer. Although memory requirements are not great, the calculationally intensive nature of the compressible flow equations suggests using a super computer. Since both the 1-D and 2-D codes were originally written for a CRAY computer, it is suggested that this super computer be used.

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