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ADIABATIC COMPRESSION TESTING I – HISTORICAL DEVELOPMENT AND EVALUATION OF FLUID DYNAMIC PROCESSES INCLUDING SHOCK-WAVE CONSIDERATIONS

ABSTRACT: Adiabatic compression testing of components in gaseous oxygen is a test method that is utilized worldwide and is commonly required to qualify a component for ignition tolerance under its intended service. This testing is required by many industry standards organizations and government agencies. This paper traces the background of adiabatic compression testing in the oxygen community and discusses the thermodynamic and fluid dynamic processes that occur during rapid pressure surges. This paper is the first of several papers by the authors on the subject of adiabatic compression testing and is presented as a non-comprehensive background and introduction.

Introduction

The compressed gas industry and government agencies worldwide have utilized one primary test methodology for qualifying high-pressure valves, regulators, and other related flow control equipment for gaseous oxygen service. This test methodology is known by various terms including adiabatic compression[3] testing, gaseous fluid impact[4] testing, pneumatic impact testing, and BAM[5] testing as the most common terms. Generally speaking, adiabatic compression is widely considered the most important ignition mechanism for directly kindling of a nonmetallic material in oxygen and has been implicated in many fire investigations. The temperature rise by near-adiabatic compression has commonly been calculated by assuming

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[3] While various terms are used for the type of testing discussed herein, adiabatic compression testing is the term that will be used most frequently in this document. This term is chosen not because it is an accurate description, but because it is used most widely within the industry. It is actually the methodologies irreversibility's and non-adiabacity that this research program is evaluating.

[4] "Gaseous Fluid Impact" is the officially balloted description in **ASTM International Test Method G74** "*Standard Test Method for Ignition Sensitivity of Materials to Gaseous Fluid Impact*:" [5]

[5] BAM stands for Bundesanstalt für Materialforschung und – prüfung and is the German Federal Institute for Materials Research and Testing where the test methodology originated in the 1950s. The test method was also implemented by the National Aeronautics and Space Administration (NASA), in a somewhat different form, after the 1970s.

ideal gas behavior through the polytropic equation[6] considering isentropic behavior (reversible and adiabatic).

The predominant test methodology that is normally utilized and a means of evaluating the thermal profiles (i.e., temperature vs. time) for various test systems has been discussed in another publication [1] by these authors. This paper outlines the historical development of the test method and discusses some of the fluid dynamic processes that are being considered in an effort to fully describe the test. This paper is not comprehensive but instead attempts to broadly outline the historical development of the test method and especially discuss the approaches that have been used by practitioners to estimate the temperatures produced during a pressure surge cycle when the test is conducted. This temperature profile and whether it differs from one test system to another is of primary interest to the authors and will be the subject of both measurement and modeling in subsequent papers on this subject.

Historical Development and Background of Adiabatic Compression Testing:

The hazard associated with compression heating of oxygen in components and systems has long been known in the industry. The 1983 keynote address by Robert Neary [2] during ASTM G04's first technical symposium celebrated the release of ASTM Standard Guideline G63 [3], which was a guide for selecting materials for oxygen service. Mr. Neary celebrated ASTM Guide G63 as, "***the industry's first guide***" for evaluating materials for oxygen service. In this paper Neary reports that the Compressed Gas Manufacturers Association (CGMA, later shortened to the Compressed Gas Association or CGA) formed an Oxygen Regulator Research Committee in 1921 due to fires caused by adiabatic compression of oxygen. Neary reported that the first product of the newly formed CGMA industry committee in 1923 was a report on

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[6]The temperature produced by adiabatic compression is usually calculated using isentropic relationships assuming that the oxygen behaves like an ideal gas and that the compression process is sufficiently rapid that heat transfer does not occur during the short time of the pulse (i.e., essentially adiabatic). The form of the equation normally used to calculate the final temperature is:

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

where: T_f = Final Temperature (abs)
T_i = Initial Temperature (abs)
P_f = Final Pressure
Pi = Initial Pressure
k = ratio of specific heats for oxygen (1.4)

oxygen regulator fires that recommended two principle test methods, "*the combustion (autoignition) test*", and "*the heat of (adiabatic) compression*" test. Neary indicates that after the 1980 release of ASTM Guide G63, the ASTM committee's focus shifted to the release of ASTM Standard Test Method G72, "*Determination of Autogenous Ignition Temperature of Liquids and Solids in a High-Pressure Oxygen-Enriched Environment*" [4] and ASTM Standard Test Method G74, "*Test to Determine Ignition Sensitivity of Materials to Gaseous Fluid Impact"* [5]. These standards essentially became the first industry-wide implementation of the 1923 recommendations of the CGMA Oxygen Regulator Research Committee. *However, while the standards were a positive step toward the implementation of test methods to improve oxygen safety, the discussions in the standards do not go beyond the common isentropic relationship (eqn. 1) for specifying the temperature of the compressed gas.*

Werley [6] provides an insightful review of adiabatic compression testing in his 1993 paper, "*A Perspective on Gaseous Impact Tests: Oxygen Compatibility Testing on a Budget"*. In the background section of this paper Werley describes the substance of the ASTM G04 committee discussion pertaining to ASTM Standard G74's development. He indicates that in the early 1980's when the committee was drafting G74, the members were aware of test apparatus utilized by companies such as AIRCO, RegO, AGA, and Circle Seal as well as government testing agencies such as BAM and NASA. He points out that some practitioners felt that adiabatic compression testing "*ignited everything*" and other practitioners felt that the test was insensitive and only ignited materials like PTFE at elevated pressures. Werley indicates that in the early 1980's the only active members of the ASTM G04 committee that conducted this test were NASA, AGA, and Circle Seal and that among these institutions NASA had conducted more extensive work. As a result, the ASTM G04 committee chose to depict the NASA apparatus in the standard; but, the test parameters were selected to be consistent with the other apparatus capabilities as well.

Adiabatic compression ignition was alleged in many fires in the industry throughout the years and was an ignition mechanism utilized in much material and component testing. In 1993 Ulrich Koch reported in a paper on Oxygen System Safety [7] the results of five different fire investigations. He admits in this paper that, "*the primary emphasis is on adiabatic compression, which has been identified as a significant but often overlooked cause of oxygen fires*." In Koch's opinion, adiabatic compression should have been implicated in even more fires than it had been. In this paper he provides the common methodology for calculating the theoretical

maximum temperature by use of the isentropic relationship. In 1997 Koch [8] remembered the Robert Neary reference to the 1923 CGMA paper that implicated adiabatic compression as a "*common cause*" of fires. Koch goes on to identify adiabatic compression as the ignition source in several other fires including US Navy training facility dating to the 1970s and opines that adiabatic compression as an ignition source must be "*century-old knowledge*" since Linde, Hampton and their peers, who developed air-separation technology to produce oxygen, must have "*understood the essentials of what would cause an oxygen fire*".

The ASTM G 74 test system was heavily utilized by NASA-WSTF [9], who at that time was the only NASA center that conducted adiabatic compression testing consistent with G 74. In the early 1990's, at the request of the Circle Seal Corporation, Wendell Hull & Associates, Inc. (WHA) developed a similar test system patterned after the NASA system but also consistent with the predominant industry standards [10] in Europe. In Europe, at that time, the test systems of prominence were operated by BAM [11, 12] and Air Liquide (CTE) [13-16]. Dr. Binder at BAM provides a good description of his test system in his 1995 paper [12] and includes the statement that, "*This method has been well established in evaluating oxygen equipment and is required in Germany by DIN, CEN standards, and even by ISO standards*." Wegener and Binder [11] describe the temperature rise in the compressed gas and the influence on ignition as follows:

> *"A compression of oxygen at 20°C from 0.l to 2.5 MPa yields a temperature rise to 410°C (this can easily be calculated according to Poisson's equation). This temperature is higher than the ignition temperature of most organic substances, so that gaskets (as seat gaskets, stuffing boxes and piston rings), lubricants, hydraulic fluids, and so forth are ignited and can burn in an explosive manner if exposed to an adiabatic compression of oxygen. Such oxygen impacts may happen, for example, in pipes if shut-off fittings under pressure are opened too rapidly or in reciprocating compressors. In general, however, such compression processes do not take place adiabatically so that temperature peaks are obtained that lie between the initial temperatures and theoretically calculated maximum temperatures."*

The temperatures indicated by Wegener and Binder are easily obtained through use of equation 1, as provided earlier.

Air Liquide has made significant contributions to the way in which adiabatic compression testing is currently being carried out and to the development of criteria to increase the test severity and improve the reliability [11-16]. Barthelemy et.al, report in 1988 while discussing flexible hose ignitions that, "Another (ignition) explanation proposed was an *"adiabatic compression" process;*

when a gas is compressed rapidly, it increases in temperature. The theoretical final temperature when oxygen is compressed, assuming the process is adiabatic (for example, assuming no mixing with hose gases, no shock waves, and no heat transfer to the hose or containers walls), is calculated from the (familiar isentropic relationships)." The assumptions provided by Barthelemy are commonly assumed and considered valid for very rapid compression processes. However, the assumption of "*no shock waves*" is important and will be further discussed later. Indeed, Air Liquide performed a shock wave analysis of the compression process in 2000 [17] that will be discussed in a later section.

Air Liquide recognized in 1989 that results could differ between test laboratories and therefore altered its internal test procedures to be more severe than the predominant standards and achieve more conservative results [13]. The work reported in this paper was foundational to several changes that were eventually incorporated in the predominant International Standards [18] and European Norm Standards [19] including a test pressure of 1.2 times the working pressure of the component and installation of the test article downstream of an impact tube of specific dimensions[7]. This research along with the advocacy of Air Liquide led to the very wide subscription of the industry standards to these provisions. Today, most industry standards that require adiabatic compression testing (see Table 2 in reference 1) utilize the test parameters that originally appeared in the 1983 version of ISO 2503 as modified by the recommendations of Air Liquide after this work was published. The only other industry standard that was not modified with these provisions was ASTM G74, which was maintained by NASA-WSTF. Further, no industry standard provided any guidance pertaining to the calculation of the temperature or thermal energy in the compressed gas other than the isentropic relationship (equation 1).

Adiabatic Compression testing has been utilized heavily by NASA [20-23]. NASA-WSTF used the ASTM G74 test methodology for individual nonmetallic materials and valves for both material selections, batch qualification of non-metallic materials, and to evaluate components such as regulators and Teflon®-lined flexible hoses [9, 21, and 22]. Stradling [9] provides an early (1983) discussion of the NASA uses for ASTM G74 and as the NASA designer/originator

[7]Test articles normally installed on a cylinder are tested at the end of a 5-mm inside diameter tube that is 1-meter long. Test articles normally installed on a manifold are tested at the end of a 14-mm diameter tube that is 750-mm long.

of the test method provides his insights into the usefulness of pneumatic impact testing[8]. Hirsch et.al, [21, 23] provide a history of how NASA used the test method between the mid-1970s up through 2003. While the statistical approach utilized within NASA for testing non-metallic materials has been questioned (discussed below), Hirsch points out that as long as statistically rigorous methods are utilized in the collection of ASTM G74 data, the results are not only meaningful; but, even produce a strong correlation between the 50% reaction pressure[9] and the Autogenous Ignition Temperature (AIT) [4] of the material being tested [23].

As mentioned above, variability observed in the non-metallic material test data produced by ASTM G74 in the late 1980s and early 1990s caused NASA-WSTF to conduct several test programs to study the statistical aspects of quantal (go/no-go; ignition/no-ignition) type testing [26-28]. This testing changed the way that NASA utilized ASTM G74 testing due to its clarification of the statistically low confidence produced by the manner in which the tests were being performed. Normally, the ASTM G74 testing was performed to rank a material according to the pressure at which a non-metallic material achieves zero (0) reactions in 20 successive pneumatic impacts[10]. Hirsch summarizes the problem well, "*An analysis of the cumulative binomial probabilities for the ASTM G74 procedure indicated that for a probability of reaction of 0.05 (assumed) for a single trial, the probability of obtaining zero reactions in the 20 trials prescribed by the standard logic is about 36 percent [23]. As a result, the lack of precision with the G 74 test logic could be potentially misleading when results were used to rank or qualify materials for oxygen service*."

For the purposes of this background, however, the statistical aspects of ignition are not as interesting as the thermodynamic principles discussed in this research. In 1988 Schmidt et.al, [26] attempted to evaluate the test methodology by using an instrumented test chamber. In this instrumented test chamber (pressure surge volume) they included a fast response pressure transducer to record the pressure rise rate, a photocell to record the light emission from an ignition, a special fast-response thermocouple called an "*eroding bead thermocouple*[11]" [29] for

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[8]Stradling was a charter member of the ASTM G04 committee and worked alongside Robert Neary and others to propel this ASTM committee and its standards into worldwide prominence in oxygen.
[9]The 50% Reaction Pressure is the pressure at which 50% of the test samples react as determined by a statistically rigorous methodology known as the Bruceton Up-Down method [23-24].
[10]In reality, a "passing" pressure level was achieved by either zero (0) reactions in 20 successive pneumatic impacts OR 1 reaction in 60 pneumatic impacts.
[11]This type of thermocouple is made by the NANMAC Corporation and is fabricated of very fine films of two metals, such as chromel and alumel films for Type K, encased in an aluminum-oxide and stainless sheath. The thermocouple sheaths are open at the end so that the end can be polished thereby "smearing" the two metal films

measuring the temperature produced in the pressure surge. Schmidt proposed the following ignition mechanisms might be active during the pressure surge to ignite a non-metallic material located at the dead end of the pressure system:

1) Adiabatic compression of the oxygen in the test chamber before impact,
2) Adiabatic compression of a bubble of gas trapped within the test material,
3) Heating of the test material by mechanical compression or mechanical shear,
4) Interaction of shock waves with the test specimen,
5) A combination of several of the above mechanisms.

For our purposes, the potential for shock wave development during the compression process is of interest since the gas velocity and temperature are not the same behind a shock wave as behind a compression wave having the same pressure ratio [30]. Indeed, shock processes are fundamentally different form isentropic compression and would lead to different features of a model seeking to define the state conditions of the test gas. The NASA interest in shock wave development within the compressed gas was heightened during the testing by Jannoff et.al, [22], Pedley et.al, [31], and Forsyth et.al, [32] who had all observed brief flashes of light within tubes undergoing a compression process sometimes one or two-hundred milliseconds before a combustion event developed[12]. In 1987 Pedley discounted these flashes as ignition due to inadvertent contamination in the tubes they were testing. Jannoff and Forsyth[13] however evaluated the phenomenon further due to the unusual nature of the light emitted when the installation of pre-cleaned, empty, tubes also produced light emission on several occasions. Forsyth theorized that the light emission could be due to the emittance of sodium or potassium spectra, in visible wavelengths, from the pre-cleaned stainless tubes. He indicated that, "*a related cause is a phenomenon known as "double electron transfer", or the release of energy in*

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together to form a junction. The film thickness once polished develops a junction with a time constant proportional to the polished film thickness. In certain applications the time constant is in the microseconds according to NANMAC. They are referred to as "eroding bead thermocouples" since in an application measuring combustion temperatures they will erode or burn but will continuously re-make their junction. Based on WHA experience and discussions with Dan Nanigian, who holds the patent for these thermocouples, they do not work well in the application envisioned since a film of cold gas forms over the junction interfering with the sensation of heat in the compressed gas. The WHA tests with these thermocouples included different shapes (i.e., spherical ends and wedge shaped ends) in an effort to resolve this problem. However, results similar to NASA-WSTF were achieved where only a small temperature rise in the gas was measured. The principle of measurement for these thermocouples is provided in reference 34.

[12]Usually the lower the pressure the longer the period between the flash of light and the development of a visually observed combustion front.

[13]Personal communication with Mr. Forsyth revealed that he had performed such rigorous cleaning and cleaning verification of his test tubes that he was confident that the phenomenon was not due to combustion of a contaminant within the tube.

the form of photons resulting from electrons in the closely packed oxygen molecules changing states". He goes on to indicate that this phenomenon has been theorized to occur in oxygen at pressures above 69 bar. He said that, "*despite exhaustive efforts to characterize the emmittance, including installation of band pass filters of various wavelengths in front of the photocell, the detection of the phenomenon was too inconsistent to characterize*".

Jannoff et.al, [22] theorized that the light flashes resulted from shock ionization of the oxygen and used band-pass filters corresponding to the ionization wavelengths of 410 nm, 440 nm, and 480 nm which corresponded to transitions in the molecular structures of 01, 011, and O_2+, respectively. They captured the flash on high-speed film and provided a series of frames that demonstrate a flash lasting about 24 msec in the visible-light spectrum. Their use of the three band-pass filters indicated above along with a high-pass, > 700 nm, infrared filter resulted in his concluding that the flash of light contained all three wavelengths expected from the shock ionization of oxygen. They further indicated that the flash event contained little, if any, infrared emission and contained only wavelengths of 700 nm and below. They ultimately opined that the flash could be attributed to the shock ionization of oxygen during the compression process where pressurization rates are fast. They theorized that the shock ionization of the oxygen may play a role in the ignition process lowering the required activation energy for ignition and making the oxygen more active. The pressurization rates where these flashes were studied were on the order of 14 msec, the fastest attainable with the WSTF system. By comparison, the pressurization rate where the light flash was observed by Forsyth was 20 msec. Since Jannoff's research involved the ignition of flexhoses by rapid compression, and since ignition of flexhoses by pneumatic impact was also observed at pressurization rates of 200 msec, Jannoff et.al, concluded that adiabatic compression of the gas probably provided the primary thermal energy for the ignition process and they related the temperature rise to the isentropic relationships.

The NASA-WSTF G74 evaluations [26-28] all ultimately concluded that the thermal energy in the compression process was produced by a standard isentropic compression of the gas rather than by shock wave influences. Schmidt et.al, state that, "*Because the ignition occurs late in the pressurization cycle, shock waves, of which there is evidence only in the first 5 ms of pressurization, are probably not responsible. Further evidence for this conclusion comes from the actuation pressure study that suggests that relatively rapid pressurization does not favor ignition*." Schmidt et.al, had observed that "*the pressure-time curve measured by the dynamic pressure transducer was always steepest in the first 3 to 5 ms, indicating possible incipient*

shock wave formation". Thus they evaluated the influence on the valve opening time on the ignition frequency and ultimately concluded that "*the frequency of ignition in the instrumented chamber was higher when the valve opening speed was slower*". However, the range of opening speeds for the impact valves they used were 1.6 to 6.85 msec[14], which are not considered substantially different when compared to the ~50 msec pressurization time normal to the ASTM G74 procedure and assumed to have been used by Moffett based on the pressure rise graphs shown in his paper.

Jannoff et.al, [28] observed that by increasing the volume of compressed gas between the high-speed valve and the test sample significantly increased the probability of ignition of the test sample by a pressure surge. He also showed the ignitions were achieved reliably at 180 msec pressurization rates even though the reaction frequency decreased from the higher frequency at 18 msec pressurization rates. These observations were related by Jannoff to the theoretical temperatures produced by isentropic compression of the gas.

<u>*Shock Wave Heating or Isentropic Compression Heating:*</u>

The role of shock waves in a pressure surge consistent with the predominant test systems utilized today is still unknown. It is understood that the NASA project funding was limited and did not allow for research to be conducted much beyond that stated above. However, the fact that light emission was observed on at least three separate projects in pre-cleaned, empty stainless tubes, and that band-pass filters detected the emission at wavelengths consistent with shock-ionization of oxygen, indicates at a minimum that further evaluation of shock processes would be appropriate.

The present research intends to further evaluate this question empirically by appropriate tests in the future. However, since the influence on the thermal profile applied to a test article could be substantial, depending on whether the shock is weak or strong, the following brief background on shock wave processes pertaining to temperature rise in the gas was developed. Whether a fully coalesced shock wave can be produced in the process under consideration is uncertain;

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[14]Later studies by Moffett et.al [26] reported valve opening times from 7.8 to 16.4 msec. The actual pressurization times were not reported. Jannoff et.al, [27] reported pressurization times of 18 to 180 msec. Jannoff also reported that, "*In the method currently used by NASA, the pressurization time is between 50 and 60 msec.*" He indicated that the 18 msec pressurization time was the fastest that could be achieved in the system, although the system Jannoff used was larger in volume than the one used by Moffett or Schmidt. The 180 msec pressurization time was accomplished by placing a metering valve in the line between the high-speed valve and the test specimen. He showed the ignitions were achieved reliably at 180 msec pressurization rates even though the reaction frequency decreased from the higher frequency at 18 msec pressurization rates. The metering valve would be expected to significantly degrade a coalescing shock wave.

but, based on the NASA experiences, consideration of even weak shock processes should be evaluated as part of this research. Indeed, the question of shock processes has been raised by other oxygen practitioners, as indicated by Ducrocq et.al. [17].

In 2000 Air Liquide presented a fluid flow analysis of the gaseous impact test conducted at CTE [17] which considered the system as a shock tube. In this research the investigators used both one and two-dimensional numerical computer codes to evaluate the reason for the pressure overshoot observed so frequently in the pressure-time data for these tests (see Figure 1 discussed in reference 1; note the pressure oscillation on each test system). The most common explanation for this overshoot is an under-damped transducer responding to a step input, as shown in Figure 2 (reproduced from reference 33).

The Air Liquide researchers sought to explain the behavior of these pressure transducers instead through the use of flow processes considering the superposition of running compression/shock wave(s) and reflected expansion or rarefaction wave(s), as in a typical shock tube analysis. They used a one-dimensional numerical simulation code and successfully predicted the general shape of the oscillating pressure pulse both in the overshoot amplitude and the order of the oscillation frequency. Their simulation predicts the overall shape of the pressure oscillation through superposition of multiple compression/expansion wave interactions. Significantly, this approach considers the entire system design including the driving gas accumulator, the tube connecting the accumulator to the high-speed valve, and the impact tube to predict the transient pressure history in the system from a step change (i.e., opening of the high-speed valve). They point out that differences in the pressure oscillation should be observed for differently designed systems. By reference to Figure 1, this is exactly what WHA has observed during its testing at the different laboratories [1]. In fact, the pressure-time history appears to be unique for each system tested thus far.

The Air Liquide approach also allowed for a temperature history to be predicted utilizing one-dimensional shock tube theory; however, very steep temperatures (> 2500 K) were predicted as a result of the propagation of the normal shock. Temperatures of this magnitude are not expected; otherwise, ignition of nonmetallic test samples would occur during testing with much higher frequency. Further, the Air Liquide researchers attempted to measure the temperature rise with standard thermocouples and measured peaks of approximately 520 K (247 ^{o}C). Because of the lower temperature measured with thermocouples, they also used a two-

dimensional simulation program to study the influence of mixing due to vortex generation during the reflection of a shock wave at the end of the impact tube. They theorized that this condition would mix the hot "shocked" gas with the cooler gas along the boundary layer of the tube. The result of this simulation, for their conditions (200:1 pressure ratio), predicted that the gas moving along the axis was cooled to approximately 600 K while the gas in the hot plug moving along the wall was still approximately 1357 K. These temperatures are greater than those measured; but, have decreased as expected.

Certainly, a shock wave analysis might be capable of explaining some features of the transient process such as the pressure-time history of the system; and, if valid, would contribute to the thermal energy of the compressed gas. WHA has observed additional support for this approach through its temperature measurements as shown in Figure 3 (see reference 1 for measurement details). This figure depicts the response of a thermocouple array having bead diameters of 0.013-mm (0.0005-inch), 0.025-mm (0.001-inch), and 0.051-mm (0.002-inch) placed at the dead end of a volume being rapidly compressed. Each of these thermocouples, to varying degrees, seems to exhibit a tendency to respond thermally to the pressure oscillation being recorded by the dynamic pressure transducer. This is especially true for the 0.013-mm diameter thermocouple. Clearly, if the oscillation on the pressure transducer were merely an under-damped response of the transducer to the step pressure input, the thermocouples would not be expected to record a corresponding temperature oscillation that rises and falls somewhat in general agreement with the pressure oscillation. While this does not indicate that a shock wave produced the thermal variations, it does support the conclusion that the pressure oscillation may be real and that an explanation for this profile should be part of the overall physical model that is developed during this research.

A review of shock-tube processes was undertaken to evaluate the nature of the physical phenomenon that might develop during an adiabatic compression test [30, 34 – 39]. The adiabatic compression test system may be envisioned as a simple shock tube with the high-speed valve acting as the diaphragm separating the high-pressure driving gases from the low-pressure driven gas. In this case, however, the diaphragm opening time is much longer and on the order of 10-15 ms as compared to diaphragm rupture times of 600 microseconds common to shock tubes [30].

In a simple shock tube the processes may be envisioned as shown in Figure 4 [34, 37]. These processes may be imagined, to some extent, for the adiabatic compression test. In a shock tube, when the diaphragm ruptures both a shock and expansion wave are generated. The shock wave travels into the low pressure gas (driven gas section) and the expansion wave travels into the high pressure gas (driving gas section). A contact surface is also formed across which the pressure and velocity are constant, but the temperature and density (hence the Mach number) are different. In Figure 4, illustration “A” shows the condition just prior to diaphragm rupture. Illustration “B” shows the condition at time = t1, where the shock wave and contact surface have traveled a distance into the driven gas section and have influenced the gas properties according to the generalized temperature and pressure graphs shown. In illustration B the movement of the expansion waves is also shown as the pressure is disturbed in the driving gas section to depress the total pressure somewhat. The expansion waves move into the driving gas chamber at the velocity of sound for the undisturbed medium, region 4. The shock wave moves into the driven gas, region 1, and depending on the initial pressure ratio across the diaphragm may accelerate to speeds greater than the speed of sound of the undisturbed driven gas.

When the shock wave encounters the end of the tube section it will reflect at more than twice the magnitude of the incident pressure step. The expansion waves will also reflect when they encounter the end of the driving gas section and will travel at the velocity of sound of the medium plus the medium velocity. The conditions for reflection and the resulting change in pressure are illustrated in “C” in Figure 4.

It was the superposition of some of these dynamics that Air Liquide argued caused the pressure oscillation observed. However, since the high-speed valves do not open as rapidly as a diaphragm rupture, these processes cannot be imagined to proceed completely as described. Donald White [30] indicates that in reality even the rupturing of a diaphragm, fast though it is, would be expected to produce a series of compression waves which must coalesce into a shock wave at some distance from the diaphragm rupture. If that is true for a diaphragm rupturing in 600 microseconds, then it is certainly of greater influence for a valve opening in 10-15 milliseconds. The process described by White is illustrated in Figure 5.

If it is assumed that a shock wave is formed by the coalescence of multiple compression waves that have been formed by the rupturing of the diaphragm or the opening of a valve, then White

argues that the shock will form at a point as shown in Figure 5. White argues that as the diaphragm is rupturing a series of compression waves are sent out, each one heating the gas by compression as the individual disturbances are traveling into the driven gas section. Since each compression wave heats the gas slightly, the speed of sound for the next compression wave is higher and therefore that compression wave will have a slightly higher velocity. Each compression wave produced as the diaphragm is rupturing travels at a slightly faster velocity than the last. Eventually each of these compression waves will coalesce with the first and if the magnitude of the initial pressure ratio across the diaphragm is great enough and as long as the driven section is long enough, a shock wave will form.

Figure 5 illustrates this process in a 3-dimensional depiction. The driver and driven sections are shown along with their respective initial pressures. The time axis increases into the page showing the change that occurs after the diaphragm ruptures. Each time step is illustrated along with the associated change in pressure and movement of individual compression waves into the driven section. The development of a contact surface and the movement of the expansion into the driver section are also illustrated starting at the time the diaphragm is caused to rupture. The individual compression waves are imagined to coalesce as shown in the diagram after several time steps have occurred. Each compression wave is moving faster than the last due to the increase in local gas temperature caused by the previous compression wave. Over time, these compression waves catch the first and strengthen it until a fully developed shock forms, if the driven section is long enough. Once the shock coalesces a new contact surface and expansion wave are formed as new disturbances in the driven gas. At this point in the flow system, the usual properties as illustrated in Figure 4 again apply where, with reference also to Figure 5, $p_2 = p_e$ just as $p_3 = p_c$; but, $T_2 \neq T_e$ and $T_c \neq T3$. At this point in time, $T_1 = T4$ but $T_2 \neq T_c$ and now $P_2 \neq P_3$. After the shock wave coalesces, the process is no longer considered isentropic since part of the mechanical energy is converted irreversibly to heat by the shock wave.

White's model allows for the calculation of the time required for the shock wave to build up through successive compression waves, one catching the other; if the temperature of the compressed gas is calculated in small pressure steps by equation 1 and the sonic velocity is calculated by means of the usual relationship for local gas properties:

$$a^2 = \frac{k \cdot p}{\rho} \qquad (2)$$

where: a = local speed of sound,
k = ratio of specific heats (Cp/Cv)
p = local gas pressure
ρ = local gas density

The model described by White is essentially that which Becker developed, described in detail by Lewis and von Elbe[15] [36] in the formation of a shock wave in a long tube. The relationships developed here will allow a comparison of the temperature from a shock to be compared directly to isentropic compression. In the shock wave there appear entirely different relationships of temperature and pressure than those governing the usual adiabatic (isentropic) compression.

If the unit of mass is compressed in an ordinary isentropic manner, which may be envisioned as Becker did by enclosing it in a cylinder and moving an imaginary piston against it sufficiently slowly so that the pressure, p, throughout the gas is at each moment is equalized and smaller than the pressure on the face of the piston by an infinitesimal amount; then the increase in the internal energy, ΔE_u, by the change in volume, dV, would be shown in equation 3 [36]:

$$\Delta E_u = \int_{v2}^{v1} -p\, dv \qquad (3)$$

This is the usual relationship for energy change in a unit volume by "*p-dv*" work assuming conditions are adiabatic. Therefore the energy change in the gas (ideal) and the temperature developed by compression are easily found by these familiar terms.

However, for a shock wave the different relationships of temperature and pressure must be considered and it is useful to evaluate the temperature differences that might exist as compared to isentropic compression. Becker developed his equations by considering a unit mass of gas in front of the wave having the volume v_1 and pressure p_1 before the shock wave passes and v_2 and p_2 after being compressed by the wave. In this case the work done is $p_2\,(v_1 - v_2)$, since after the establishment of the wave the pressure on the piston is always p_2. This work would both increase the internal energy of the unit mass and impart to it kinetic energy so that the change in internal energy is expressed as:

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[15]The discussion which follows pertaining to the Becker analysis is largely based on material presented by Lewis and Von Elbe [36] which discusses the model and analysis originally presented by R. Becker in *Z. Physik* Journal in 1922 (*Z. Physik* 8,321) and later *Z. Elektrochem* Journal in 1936 (*Z.Elektrochem*. 42, 457).

$$\Delta E_u = p_2 \cdot (v_1 - v_2) - \frac{w^2}{2} \quad (4)$$

where: w = the velocity change of the disturbed gas ($u_1 - u_2$) to an observer moving with the wave. To this observer, the gas enters the wave with velocity u_1 and leaves at a smaller velocity u_2.

Becker then developed his mass, momentum and energy relationships using fundamental steady state relationships as:

$$\frac{u_1}{v_1} = \frac{u_2}{v_2} \quad (5)$$

$$\frac{u_1^2}{v_1} + p_1 = \frac{u_2^2}{v_2} + p_2 \quad (6)$$

$$E_1 + \frac{u_1^2}{2} + p_1 \cdot v_1 = E_2 + \frac{u_2^2}{2} + p_2 \cdot v_2 \quad (7)$$

As can be seen, the change in energy from equation 7 is very different from equation 3 and is not applicable to flow in which the pressure and volume changes are isentropic (reversible). Becker derived equation 7 from the energy theorem for flow where resistance occurs.

By substituting values of u_1^2 and u_2^2 from equations 5 and 6 in to equation 7, one can obtain the famous ***Hugoniot*** equation for which this type of compression replaces the integral in equation 3 for isentropic compression.

$$E_2 - E1 = \Delta E = \frac{1}{2}(p_1 + p_2) \cdot (v_1 - v2) \quad (8)$$

Lewis and Von Elbe [36] point out that the physical interpretation of the mechanism by which the gas entering the wave front is compressed according to equation 8 and not according to the ordinary adiabatic relationship follows as long as it is remembered that during an isentropic compression process the compression takes place so slowly that the pressure in the unit mass control volume is at all times equal (i.e., the external force on the piston imagined above is only infinitesimally larger than the opposing force exerted by the gas). This will be the case as long as the piston velocity is small compared to the average molecular velocity (therefore the piston

velocity can be quite high in actuality as long as these conditions hold). However, when the piston velocity becomes on the order of the magnitude of the molecular velocity, the degradation of the kinetic energy of the piston into random molecular velocities (i.e., thermal energy) contributes to the internal energy of the compressed gas. For very small volume changes the Hugoniot equation reduces to the differential form of the isentropic equation, dE = -pdv.

Faeth [40], in an excellent discussion of isentropic compression, related this condition to the wave relaxation time, ***L/a***, where **L** is the length of the driven gas section and ***a*** is the velocity of sound. For isentropic properties to be valid, the rate of compression must be slow enough that the change in pressure with distance ($\frac{\delta p}{\delta x}$) is negligible. Faeth indicated that the time of compression t_c must be much longer than the quotient L/a ($t_c >> L/a$) otherwise the pressure in the driven gas section cannot be assumed to be isentropic and the pressure varies with position in the tube.

From equations 4, 5, and 6 the velocity of shock propagation into the gas at rest, $\mathbf{u_1}$, and the velocity **w** of the gas behind the wave, often referred to as the particle velocity, is found from equations 9 and 10. Equation 11 is the ideal gas law, where **n** = the number of moles per unit mass and **R** is the molar gas constant, and equation 12 relates the internal energy of an ideal gas to its change in temperature, with C_v being the average specific heat at constant volume (between T_1 and T_2), as follows:

$$u_1 = v_1 \cdot \sqrt{\frac{(p_2 - p_1)}{(v_1 - v_2)}} \tag{9}$$

$$w = (v_1 - v_2) \cdot \sqrt{\frac{(p_2 - p_1)}{(v_1 - v_2)}} \tag{10}$$

$$p \cdot v = n \cdot R \cdot T \tag{11}$$

$$\Delta E = C_V \cdot (T_2 - T_1) \tag{12}$$

From these relationships, Table 1 was presented by Lewis and Von Elbe and provides the comparison between shock temperatures and isentropic temperatures that we were seeking. As can be observed, the shock wave produces a temperature that is very different from ordinary isentropic compression for the same pressure ratio. At low pressures the magnitude is similar but for higher pressure ratios the difference is significant. ***Therefore, as a minimum, this research must evaluate the presence and strength of any shock wave that might develop***

from the rapid opening of the high-speed valve. It is considered probable that because the high-speed valve opens in a time much longer than a diaphragm ruptures that shocks do not fully coalesce before the compression waves reflect at the dead end of the driven gas section. However, certainly some compression waves would be expected to catch and strengthen the leading compression front and thereby create a pressure disturbance in the driven gas that could be similar to a partially formed shock. Leslie points out that for a 1-meter long tube and for a sonic velocity of 350 m/s the wave relaxation time, t_a = 2.8 ms. So, for a 15 to 20 msec target pressurization time as required by the present standards, $t_c \sim t_a$, and the condition for isentropic compression may not be achieved. ***Based on this result also, the presence of partial shock conditions (i.e., strong compression waves) should at least be evaluated in any model that is developed to predict the thermal profile produced by the compression process.***

Table 1 – Shock Waves in Oxygen (k = 1.4) for Different Pressure Ratios

p_2/p_1	v_1/v_2	w (m/s)	u_1 (m/s)	T_{2_shock} (K)	$T_{2\_isentropic}$ (K)
2	1.63	175	452	336	330
5	2.84	452	698	482	426
10	3.88	725	978	705	515
50	6.04	1795	2150	2260	794
100	7.06	2590	3020	3860	950
1000	14.3	8560	9210	19100	1710
2000	18.8	12210	12900	29000	2070

Reference 35 points out that the values of Cv used by Becker in these calculations are not accurate at very high temperatures, but, the essential trend is the same.

Real Gas Properties

One final adjustment to the temperatures estimated for the compressed gas in a pressure surge has been suggested by several researchers. It has been recognized that temperatures predicted by the polytropic equation (eqn. 1) and shown in Table 1 ($T_{2\_isentropic}$) are based on ideal gas behavior and overestimate the actual temperature if real gas properties were considered. Since an accurate prediction of the thermal energy in the compressed gas tube (driving gas recompression + driven gas compression) is desired in this research, then evaluation of the state of the gas during the compression process utilizing real gas relationships

and equations of state would be useful. Recently, several researchers [41-43] have adjusted the polytropic exponent ($p\,v^k$ = constant) by empirical measurements or by considering the compressibility and change in specific heats of oxygen (Leslie [41]) to predict the temperature rise using the polytropic relationship adjusted for some real gas properties. By adjusting the exponents, under very specific conditions, these researchers have shown that the temperature developed by compression of a real gas may be calculated using this simple relationship. However, the exponent derived by this approach is only valid for the specific conditions under which it was developed and is not a true equation of state for the real gas properties. Its use must be confined to the circumstances in which it was developed. For instance, Leslie reports that for the form of the polytropic equation shown in equation 13, three values of the polytropic exponent may be derived for $T_{initial}$ = 300 K and $P_{initial}$ = 100 kPa, as follows:

$$\left(\frac{T_{final}}{T_{initial}}\right) = \left(\frac{P_{final}}{P_{initial}}\right)^n \qquad (13)$$

Leslie Eqn. 1:	n = 0.2829	Ideal Gas – Ordinary Isentropic Value, k = 1.4
Leslie Eqn. 2:	n = 0.2599	Ideal gas with variable specific heats
Leslie Eqn. 3:	n = 0.2632	Real gas (van der Walls), variable specific heats

The resulting calculations, starting from the initial conditions given above, are shown in Figure 6, on a log-log chart to linearize the behavior. This figure compares two different real gas approaches to calculating the compressed gas temperature compared to the normal isentropic approach using equation 1. As is evident in this figure, the results of the calculation show that the polytropic exponent for ideal gas with variable specific heats and a real gas model using *van der Walls'* relationship and variable specific heats result in very similar temperatures, for the starting conditions chosen. At high pressures, the real gas temperatures predicted diverges from the ideal gas, isentropic, predictions.

However, approaches that simply adjust the polytropic exponent are not equations of state useful for all reasonable conditions. Barragan, Wilson and Stoltzfus [44] have derived from thermodynamic principles closed form equations of state for oxygen that do allow the calculation of isentropic compression temperatures using real-gas properties, as shown in Figure 7. This figure compares the temperatures calculated by different methods, as follows:

T_{id}* = temperature found by using the normal isentropic equation

T_{id} = temperature found by assuming the fluid is an ideal gas but that does not have a constant heat capacity over the temperature range of interest. In this case the heat capacity is allowed to vary by ordinary thermodynamic relationships.

T_{real} = temperature found with the compressibility relationship substituted into an equation of state developed for the entropy change during the compression process.

The equations of state calculations are all similar and reduce the predicted temperature by about 200 K for a pressure ratio of 100. Barragan, et.al., point out that the calculation of T_{real} considers both the heat capacity variation with temperature and the effect of pressure giving the best value that can be obtained by thermodynamic analysis. Therefore, for future papers in this series, calculation of the theoretical maximum temperature will evaluate the real gas relationships derived by Barragan, Wilson, and Stoltzfus [44].

Summary and Conclusions from Background Research

This paper sought to outline the historical development of the gaseous fluid impact (or adiabatic compression) test method and discussed some of the fluid dynamic processes involved; and to outline some of the considerations that will be evaluated by the authors in further testing and research to estimate the temperature and energy developed during a pressure surge. The temperature profile in the compressed gas and whether it differs from one test system to another is of primary interest to the authors and will be the subject of both measurement and modeling in subsequent papers on this subject. This paper sought to provide background for this research and is the first in a series of papers planned on this subject.

The second paper in this series is presented herein as reference 1; and, presents a measurement technique for the determination of the temperature profile in a typical pressure surge. Initially, the research attempted to define differences in the various test systems by the temperature profile; however, due to limitations in the ability of thermocouples to respond quickly to transient thermal changes, the presence or non-presence of shock waves could not be verified by temperature alone, as will be discussed in reference 1. Additional testing and modeling will be utilized in later research to attempt a resolution of this important question.

Based on consideration of the background discussed above, the following general conclusions have been drawn, pertaining to the estimation of temperature in the compressed gas:

1) No research that we are aware of has empirically measured the thermal energy in the driven gas section for the methodology required today by the predominant standards. Several researchers have attempted measurement including NASA-WSTF, Air Liquide, WHA, and Faeth [40] but temperatures do not compare favorably (temperatures are significantly lower) to the temperatures estimated by either isentropic or shock methods. Faeth used a unique approach, further discussed in reference 1, and has produced measurements closer to those expected than other researchers; however, his systems were larger and pressurized much more slowly than the systems under consideration here.

2) An industry consensus has not been developed as to what thermodynamic and/or gas flow processes are causing the increase in thermal energy that leads to ignition of a non-metallic material by this test. Heating by frictionless-adiabatic (isentropic) compression and shock tube methods are both alleged as the predominant processes involved. However, neither the presence of shock waves nor the irreversibility's of the compression process have been defined so that the temperatures actually produced have been determined.

3) The fact that light emission was observed on at least three separate NASA projects in pre-cleaned, empty stainless tubes, and that band-pass filters detected the emission at wavelengths consistent with shock-ionization of oxygen, indicates, at a minimum, that further evaluation of shock processes would be appropriate. On the other hand, the relatively long opening time for the valves commonly used in this test, as compared to diaphragm rupture times for shock tubes, calls into question whether a fully coalesced, or even strong, shock wave could develop in the distance between the valve and a test article (usually 1-meter). ***Therefore, the role of shock waves in a pressure surge consistent with the predominant test systems utilized today is still unknown.*** Since the existence and/or strength of a shock wave in a typical pressure surge cycle is unknown, additional testing and modeling is required to further evaluate the presence and strength of shock processes in order to determine their influence (if any) on the temperature produced in the compressed gas.

4) The following temperature predictions for the compressed gas volume that predominate in the literature can be summarized as follows:

   a. Isentropic compression calculations using ideal-gas properties produce much higher temperatures than have been confirmed by measurement.

   b. Isentropic compression calculations using real gas properties also produce much higher temperatures than have been confirmed by measurement.

   c. Adiabatic compression of oxygen using a real-gas equation of state derived from thermodynamic properties predicts much higher temperatures than have been confirmed by measurement.

   d. Shock process calculations derived from first principles predict temperatures well in excess of those measured and also exceed the predictions from any form of isentropic compression.

   e. One-dimensional numerical methods used to predict the temperatures produced in the test system by superposition of reflected compression waves and expansion waves predict temperatures much higher than have been confirmed by measurement.

   f. Two-dimensional numerical methods used to predict the temperatures produced by superposition of reflected compression waves and expansion waves that include mixing predict temperatures higher than measured but closer, within twice that measured.

5) Empirical data supports that the pressure oscillation observed in the pressure-time measurements is not due to instrumentation characteristics such as an under-damped transducer. Instead, the oscillation can be shown to produce a thermal response in the WHA thermocouples (Figure 3). Further, the Air Liquide shock model reproduced many of the essential features of the pressure-time oscillation history. Therefore, a proper understanding of the test system influence on the thermal energy should explain the pressure-time “fingerprint” developed by the test system.

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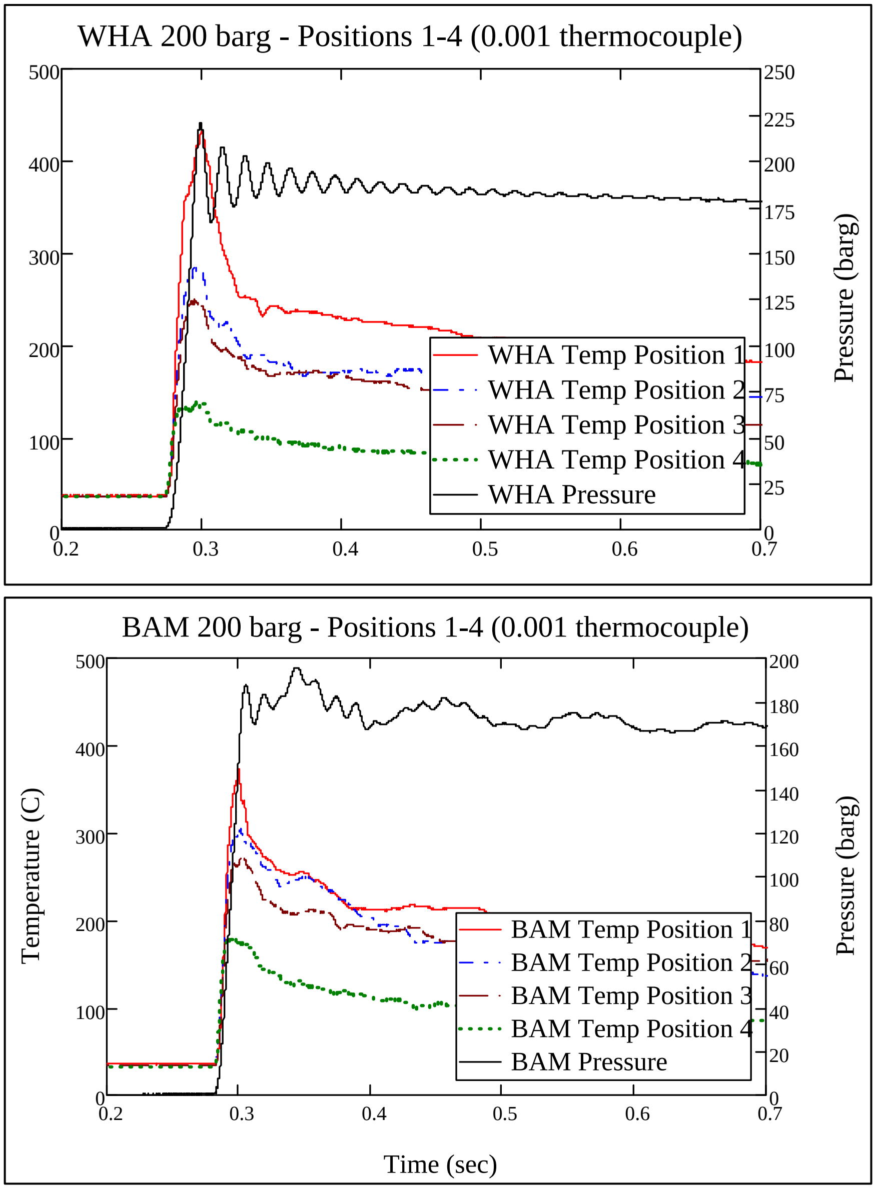


Figure 1 – WHA and BAM Pressure and Temperature Profiles

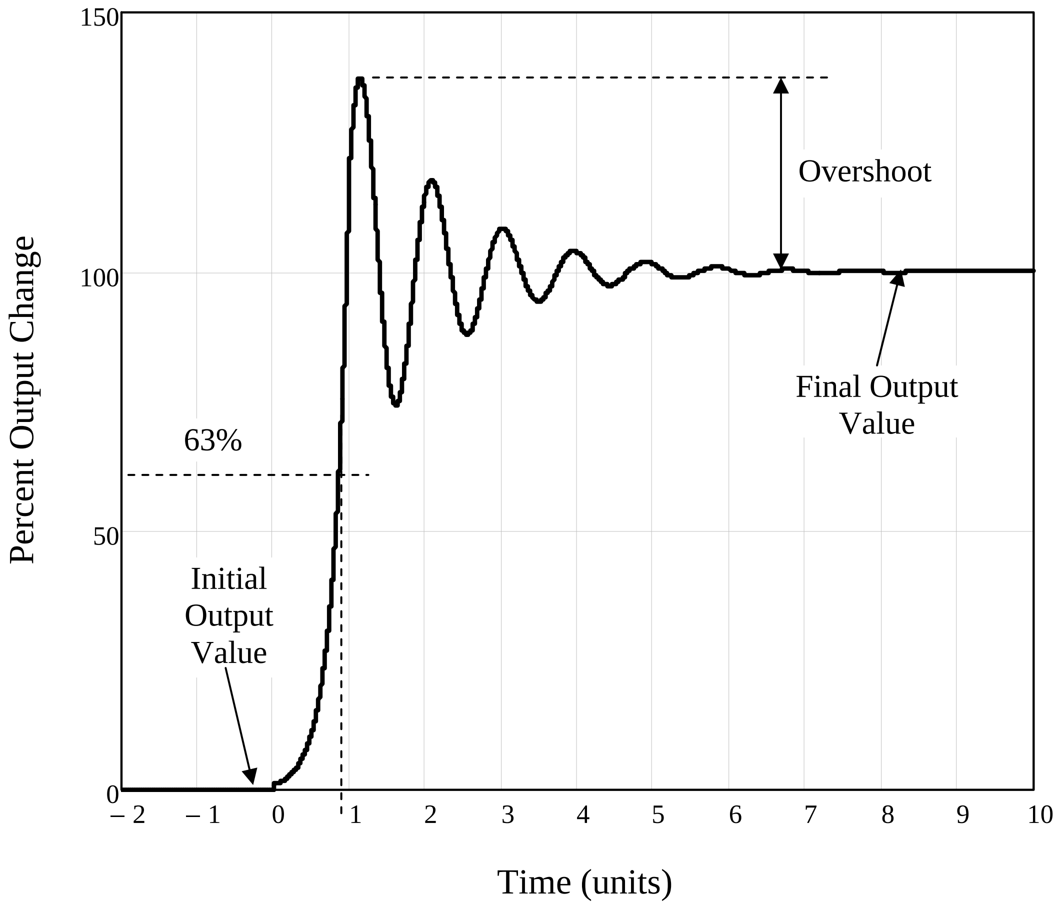


Figure 2 – Response of Under-damped Transducer to Step Change [32]

Figure 3: WHA Test - 180 barg, Test 13 - Cycle 1

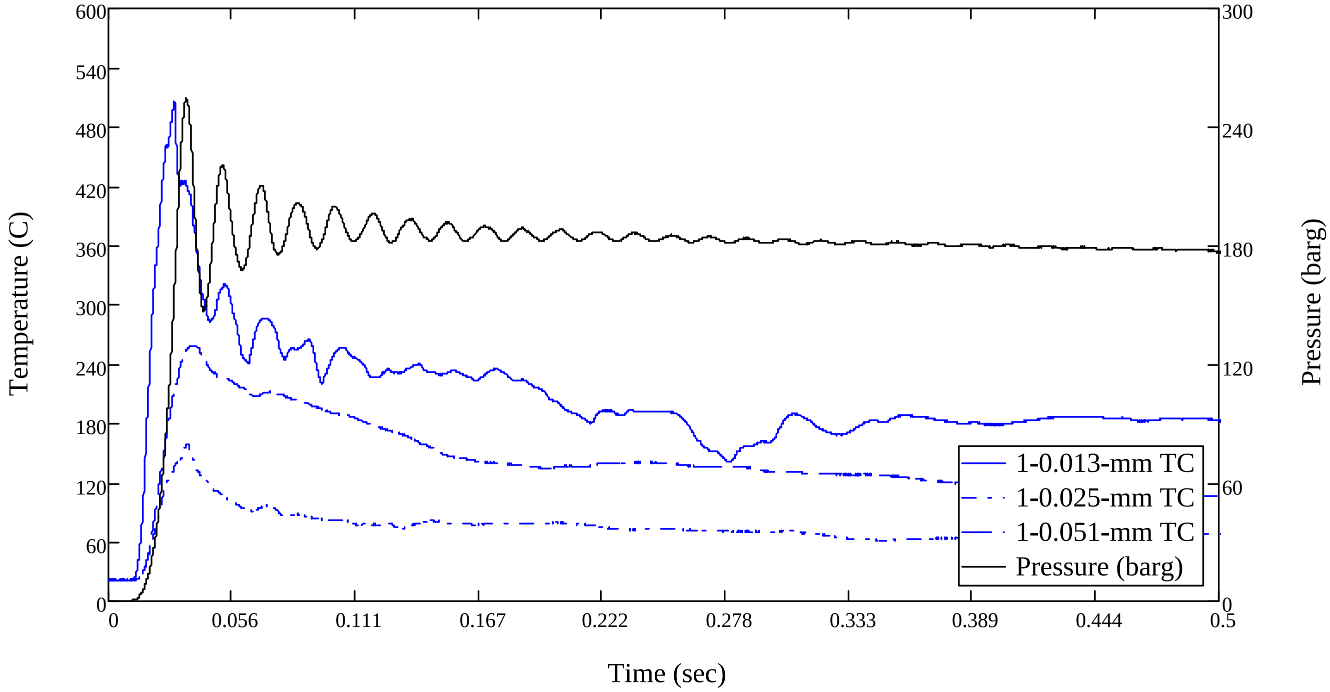
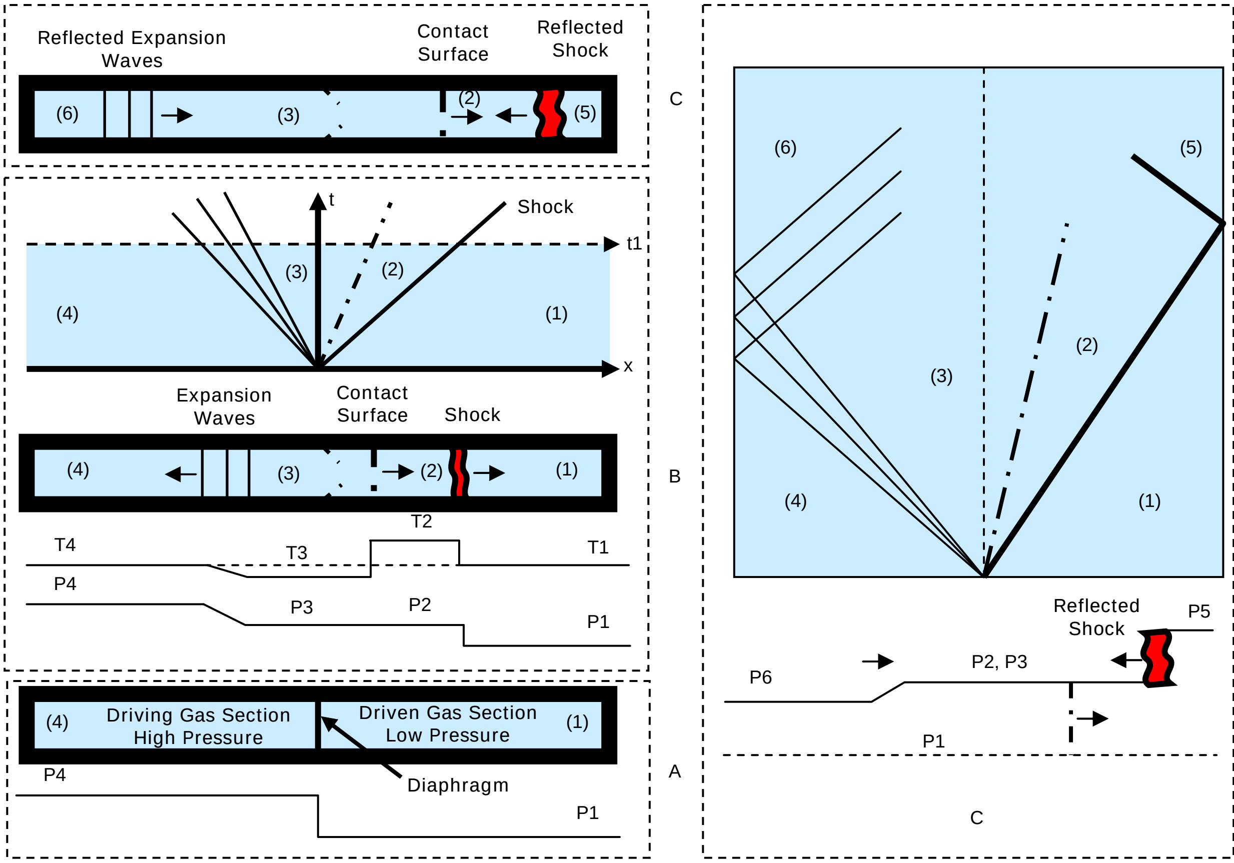


Figure 4 – Simplified Illustration of Shock Tube Processes Related to Rapid Compression



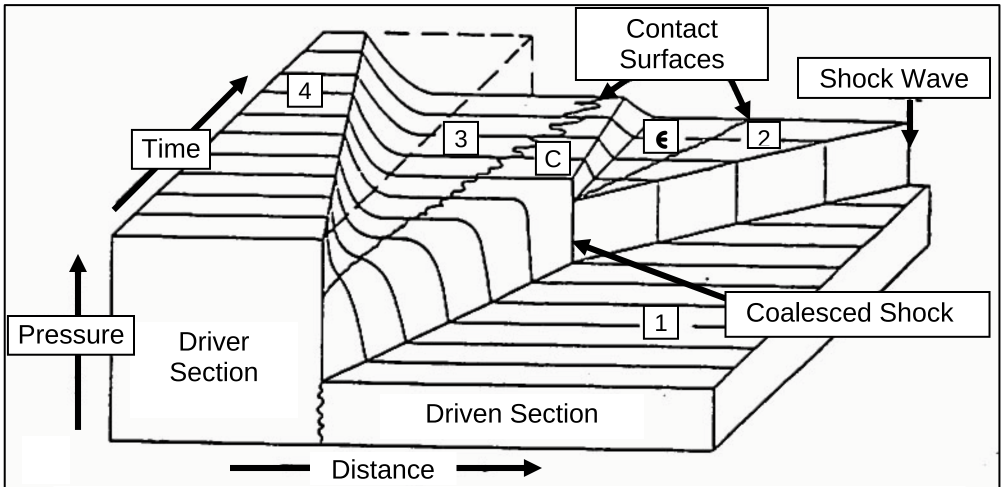


Figure 5 – Illustration of Shock Formation after Diaphragm Rupture [29]

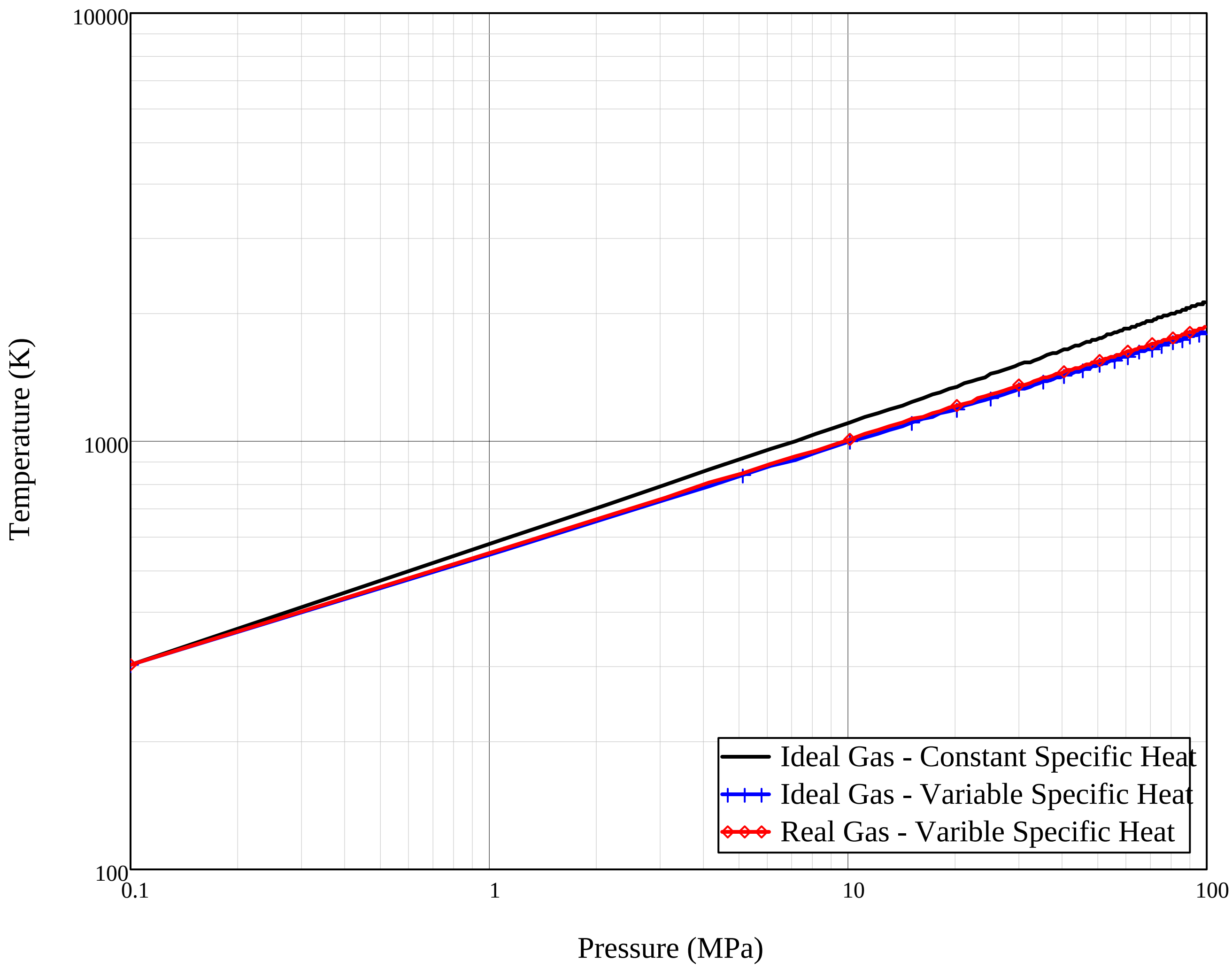


Figure 6 – Isentropic Temperature – Pressure Relations [40]

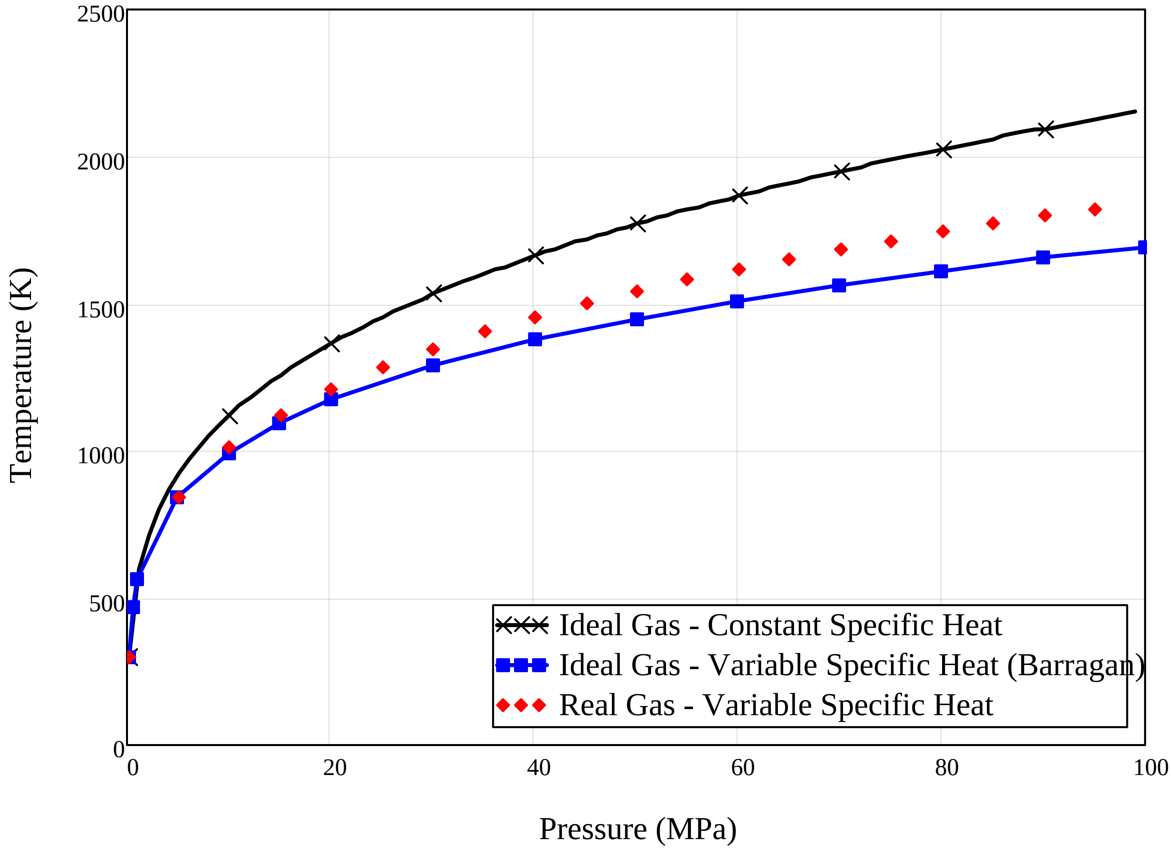


Figure 7 – Temperature for Isentropic Compression of Oxygen Using Real Gas [43]