Estimation of evaporation of previously condensed hydrocarbons in a tunnel burn experiment

Zoran Stefanoski
University of Nevada, Las Vegas

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ESTIMATION OF EVAPORATION OF PREVIOUSLY CONDENSED HYDROCARBONS IN A TUNNEL BURN EXPERIMENT

by

Zoran Stefanoski

Bachelor of Science
St. Kiril & Metodij University
Skopje, Macedonia
1996

A thesis submitted in partial fulfillment of the requirements for the Masters of Science Degree
Department of Mechanical Engineering
Howard R. Hughes College of Engineering

Graduate College
University of Nevada, Las Vegas
December 2000
The Thesis prepared by

Zorani Stefanoski  

Entitled

ESTIMATION OF EVAPORATION OF PREVIOUSLY CONDENSED HYDROCARBONS IN A TUNNEL BURN EXPERIMENT

is approved in partial fulfillment of the requirements for the degree of

Master of Science in Mechanical Engineering

Examination Committee Chair

Dean of the Graduate College

Examination Committee Member

Examination Committee Member

Graduate College Faculty Representative

PR/1017-53/1-00
ABSTRACT

Estimation of Evaporation of Previously Condensed Hydrocarbons in a Tunnel Burn Experiment

by

Zoran Stefanoski
Dr. Robert F. Boehm, Examination Committee Chair
Professor of Mechanical Engineering
University of Nevada, Las Vegas

As part of the worldwide demilitarization efforts, outmoded solid rocket motor propellant is being destroyed by burning. Often this is done on a repeated basis in a closed chamber. There is concern whether or not previously condensed materials on the chamber wall might be re-evaporated during a new burn.

The objective of this thesis is to estimate the amount of evaporation/sublimation possible for different types of organic materials during burns in a tunnel. This was carried out theoretically and compared to measurements. For the estimations, predictions of the wall and ambient
temperatures were made. The evaporation/sublimation was then estimated as bulk diffusion into the tunnel air. The results provide a method to compute the evaporation rate. Good agreement is shown for the predicted temperatures compared to the measured values, although a wide variation is shown in the experimental results. Measured concentrations of various Volatile Organic Compounds from the tunnel walls are then used to estimate the maximum concentrations in the tunnel air that could occur with complete evaporation.
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NOMENCLATURE

\( \rho \)
Density

\( \alpha \)
Thermal diffusivity

\( r \)
Variable of integration

\( A \)
Surface area of the containment chamber walls

\( A, B, C, D, E \)
Regression coefficients for chemical compound

\( C_{NAPPH}, C_A \)
Concentration of naphthalene on the chamber walls

\( C_s \)
Total concentration of the condensed materials

\( c_s \)
Concentration at the surface of the semi infinite medium

\( D_{AB} \)
Mutual diffusion coefficient of A in B, diffusion coefficient of naphthalene into air

\( h \)
Convection heat transfer coefficient

\( H \)
Heat of combustion of the propellant

\( H_P \)
Enthalpy of the propellant products of combustion at the flame temperature

\( J_A \)
Molar flux of A by ordinary molecular diffusion

\( k \)
Thermal conductivity

\( L \)
Length of the chamber

\( m_1 = M \) Mass of gas existing in the chamber

\( m_2 \)
Mass of gas in the chamber plus mass of the propellant

\( m_p \)
Mass of the propellant

\( n_A \)
Molar flow rate of naphthalene

\( N_A \)
Total number of moles of naphthalene evaporated

\( P \)
Vapor pressure

\( P_{vap} \)
Vapor Pressure of Naphthalene

\( P_2 \)
Peak pressure of the gas

\( Q_{gen} \)
Total energy generated

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\( \dot{Q}(t) \)  Heat transfer to the chamber wall
\( R \)  Specific gas constant
\( R_g \)  Gas constant
\( S \)  Surface area of the chamber walls
\( t \)  Time
\( T \)  Temperature
\( T_a \)  Temperature of the gas
\( T_{\text{max}} \)  Peak temperature of the gas
\( T_w \)  Temperature of the wall at the surface
\( u \)  Ideal gas internal energy
\( V \)  Volume of the containment chamber
CHAPTER 1

INTRODUCTION

As part of the worldwide demilitarization efforts, outmoded solid rocket motor propellant is being destroyed by burning. Many of these burns have been performed where the combustion products are contained within a sealed chamber so that the gases from the combustion can be analyzed. From test to test, there is concern whether or not previously condensed materials on the wall might be re-evaporated during a new burn, thus giving incorrect emissions data for a given test.

The objective of this thesis is to estimate the amount of evaporation (Evaporation here will be used to denote evaporation, sublimation or a combination of the two) possible for different types of organic materials. This was carried out theoretically and compared to measurements. To estimate the amount of evaporation, predictions of the wall and ambient temperatures were made as a function of time during a burn test. The evaporation was then estimated as a bulk diffusion situation into the tunnel air.
The results provide a method to compute the evaporation rate, which clearly demonstrates that condensed materials can easily vaporize from the walls following the burn process.

The results are presented for three tests carried out in the X tunnel at the Nevada Test Site. Good agreement is shown for the predicted temperatures compared to the measured values, although a wide variation is shown in the experimental results. Measured concentrations of various Volatile Organic Compounds (VOCs) from the tunnel walls are then used to estimate the maximum concentrations in the tunnel air that could occur with complete evaporation.

The model developed for this analysis considers only those mixtures where no chemical reactions occur, where the components are ideal gases or incompressible solids and the products of combustion are considered to be well mixed with the existing gas in the chamber. Further, surface tensions between various components and capillary action are ignored. In the following discussions only ideal gas mixtures and dilute gas/solid mixtures are considered. The most useful model for ideal gas mixtures is the one that assumes that every component of the mixture occupies the full mixture volume. The primary mode of heat transfer to the chamber walls is assumed to be convection.
to the chamber floor is considered to be negligible. Radiation to the chamber walls is also considered to be negligible due to the opacity of the gases following combustion.

Physical Characteristics of the Containment Chamber

The most important features of the chamber geometry are the total volume and the total surface area of the chamber (walls and floor). The walls consist of a 152-203 mm (6-8") layer of sprayed concrete over alluvium and the floor is a poured concrete pad, see Figure 1. The entrance to the chamber is a steel "containment barrier" with a negligible surface area compared to that of the overall chamber.

Figure 1. Chamber cross section
CHAPTER 2

MATHEMATICAL ANALYSES

Mass Transfer Analysis

Evaporation of a particulate solid is a fundamental process of mass transfer with a variety of natural and industrial applications. Under typical conditions, the evaporating species diffuses through a sparse or consolidated matrix of particles and enters the ambient under the influence of an externally imposed concentration gradient. The thermal (kinetic) energy drives the molecule's fluctuating state of motion. In a homogeneous fluid or solid (where the concentration is independent of the position when averaged over a distance that is large compared to molecular dimensions), this motion brings about no change in mean composition. In an inhomogeneous medium (one with a mean concentration gradient with respect to some chemical species), this fluctuating motion can give
rise to a net movement of a particular species (diffusion),
with respect to some coordinate system.

A similar process occurs during the drying of a porous
medium or a concentrated suspension such as a paste or a
photographic emulsion. During the late stages of drying,
the liquid phase forms disconnected globules that are
supported by an underlying fiber or particle network, and
diffusion occurs through the interstitial spaces and into
the dry environment.

The law of diffusion can explain this molecular
motion. Diffusion is a mode of mass transfer. Mass transfer
is the net movement of a component in a mixture from one
location to another location where the component exists at
a different concentration. Often, the transfer takes place
between two phases across the interface. Thus, the
absorption by a liquid of a solute from a gas involves mass
transfer of the solute through the gas to the gas-liquid
interface, across the interface, and into the liquid. Mass
transfer modes are used to describe processes such as the
passage of a species through a gas to the outer surface of
a porous absorbent particle and into the porous surface.
Mass transfer occurs by two basic mechanisms:
1. Molecular diffusion by random and spontaneous microscopic movement of individual molecules of a gas, liquid or solid as a result of a thermal motion.

2. Eddy (turbulent) diffusion by random macroscopic fluid motion.

Molecular and/or eddy diffusion frequently involves the movement of different species in opposing directions. When a net flow occurs in one of these directions, the total rate of mass transfer of individual species is increased or decreased by bulk flow or convective effects, which is a third mechanism of mass transfer. Molecular diffusion is extremely slow, whereas eddy diffusion, when it occurs, is orders of magnitude more rapid.

In a binary mixture, molecular diffusion occurs because of one or more different potentials or driving forces, including differences (gradients) of concentration (ordinary diffusion), pressure (pressure diffusion), temperature (thermal diffusion), and external force fields (forced diffusion) that act unequally on the different chemical species present.

Molecular diffusion occurs in solids and in fluids that are stagnant or in laminar or turbulent motion. Eddy diffusion occurs in fluids in turbulent motion. When both molecular and eddy diffusion occur, they take place in
parallel and are additive. Furthermore, they take place because of the some concentration difference (gradient). When mass transfer occurs under turbulent flow conditions, but across the interface or to a solid surface, conditions may be laminar or nearly stagnant near the interface or solid surface. Thus, even though eddy diffusion may be the dominant mechanism in the bulk of the flow, the overall rate of a mass transfer is controlled by molecular diffusion because the eddy diffusion mechanism is damped or even is eliminated as the interface or solid surface is approached.

Mathematical formulation

Now we direct attention to the possible evaporation of a condensed organic material on the wall. The analysis performed here assumes that the material of interest is naphthalene. Clearly there are several organics that are in vapor form in the tunnel following a burn episode, but we will focus only on this one. However, the general approach and the conclusions drawn can be directly applied to other substances.

In the following analysis, transport from a semi-infinite medium with a well-defined interface will be studied, where the transport is due to a concentration gradient maintained above the interface. Transport due to
natural or forced convection is neglected, and the particle
dissolution or evaporation is assumed to be limited by
diffusion. Using Fick's Law of molecular diffusion we
derive expressions for the rate of transport from the
chamber walls. We start with a proportionality between a
flux and a gradient. For a binary mixture of A and B:

\[ J_A = -D_{AB} \frac{dc_A}{dz} \]  

\[ J_A = -D_{AB} \frac{dc_A}{dz} \]  

Where, \( J_A \) is the flux of A by ordinary molecular
diffusion relative to the molar average velocity of the
mixture in the positive z direction, \( D_{AB} \) is the mutual
diffusion coefficient of A in B and \( dc_A/dz \) is the
concentration gradient of A, which is negative in the
direction of the ordinary molecular diffusion.

Many alternative forms of eqns (1) and (2) can be
used, depending of the choice of driving force or potential
in the gradient.

Vapor pressure

One of the physical properties that we can measure for
liquids and solids is vapor pressure. Vapor pressure is
defined as the pressure of the vapor of a liquid or solid
in equilibrium with the liquid or solid state. Generally
liquids have higher vapor pressures than solids. The physical process by which vapor pressure occurs is referred to as evaporation. There are several things that could influence the rate at which solid molecules become vapor.

- Polar nature of the molecules
- Surface area
- Temperature
- The concentration of vapor molecules above the liquid

The Antonie-type equation [Yaws, 1999] with expanded terms was selected for correlation of vapor pressure as a function of temperature:

\[
\log P = A + \frac{B}{T} + C \log T + DT + ET^2
\]  

(3)

\(P\)-vapor pressure, mmHg

\(A, B, C, D, E\) - regression coefficients for chemical compound

\(T\) - temperature, K

The temperature range for which the equation may be used to predict vapor pressure is denoted by the respective minimum and maximum temperatures (\(T_{\text{MIN}}\) and \(T_{\text{MAX}}\)).

Regression coefficients for naphthalene [Yaws, 1999] in the temperature range (360-480 K):

\[A = 34.9161\quad C = -9.0648 \cdot 10^2\quad E = 1.5550 \cdot 10^{-6}\]

\[B = -3.9357 \cdot 10^3\quad D = -2.0672 \cdot 10^{-9}\]
Results of the eqn. (3) for naphthalene as a function of temperature are shown in Figure 2.

Figure 2. Vapor pressure for naphthalene is shown as function of temperature.

Diffusion coefficient

The calculation of individual mass transfer coefficients in the engineering analysis of mass transfer operations requires knowledge of the diffusivity (diffusion coefficient) of the species involved. Furthermore, the calculation of the overall mass transfer coefficient also requires diffusivity data for the individual species. In fact, diffusivity is the fundamental property involved in mass transfer.
When an experimental value of diffusivity is not available for specific values of temperature (T) and pressure (P), equation (4) [Seader and Henley, 1998] can be used for obtaining the value of the diffusion coefficient.

\[ D_{AB} = \frac{0.00143T^{1.75}}{PM_{AB}^{1/2}[(\sum v_A^{1/3} + (\sum v_B^{1/3})]^2} \]  
\[ M_{AB} = \frac{2}{\left(\frac{1}{M_A} + \frac{1}{M_B}\right)} \]  

where \( \sum v \) is the summation of atomic and structural diffusion volumes.

This indicates that \( D_{AB} \) is proportional to \( \frac{T^{1.75}}{P} \). Since the diffusion coefficient varies inversely with pressure (for low and moderate pressures), values at other pressures can be ascertained from the appropriate ratio of pressures.

When an experimental diffusivity is available for temperature (T) and pressure (P) that are different from the desired conditions, a proportion represented in equation (6) is used for calculation of the needed coefficient.

At 1 atm, the experimental value for diffusion coefficient [Rolle, 2000] at 25°C (298.15 K) can be extrapolated by the temperature dependency to give the following prediction at temperature range (360-480 K) see
Figure 3. An experimental value and graphical dependence [Seader and Henley, 1998] for 298.15 K (25°C) is:

\[ D_{NAP} = 0.62 \times 10^{-5} \frac{m^2}{s} \]

\[ D_{AB}(T) = 0.62 \cdot 10^{-5} \times \left( \frac{T}{298.15} \right)^{1.75} \left( \frac{m^2}{s} \right) \]  

(6)

Based on the assumptions listed above, the ideal gas model is used for calculation of the concentration of the condensed materials in the chamber walls.

\[ C_{NAPH} = \frac{P_{VAP}}{R_g \cdot T} \]  

(7)

\( P_{VAP}\) - vapor pressure of naphthalene

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\( R_g \) - gas constant

\( T \) - temperature (K)

The total concentration of all condensed materials on the wall:

\[ C_m = \sum_{i=1}^{n} C_i \]  

(8)

Fick's first law of molecular diffusion relates the molar flow flux through the chamber air of diffusing molecules, across plane of the wall area (A), to the diffusivity and the concentration gradient at the wall. In terms of mass transfer rate by diffusion only across the plane of the chamber wall, eqn. (1) becomes:

\[ n_A = -D_A A \frac{dC_A}{dz} \]  

(9)

Based of assumptions listed above, we consider one-dimensional diffusion through a differential control volume in the \( z \) direction only; thus the molar flow rate of naphthalene species through the chamber air takes the form:

\[ n_{A,z} = -D_A A \left( \frac{\partial C_A}{\partial z} \right)_z \]  

(10)

At the plane \( z = z + \Delta z \) the diffusion flow rate is

\[ n_{A,z+\Delta z} = D_A A \left( \frac{\partial C_A}{\partial z} \right)_{z+\Delta z} \]  

(11)
If we consider accumulation of species in the control volume:

\[-D_{ab}A\frac{\partial A}{\partial z} + D_{ab}A\frac{\partial A}{\partial z} |_{-\Delta z} = A\frac{\partial A}{\partial t} \Delta z \quad (11a)\]

Rearranging eqn. (11a) and in the limit \(\Delta z \to 0\), the partial differential equation for one-dimensional diffusion is:

\[\frac{\partial A}{\partial t} = D_{ab} \frac{\partial^2 A}{\partial z^2} \quad (12)\]

This is a second order PDE in the \(z\) direction and therefore requires specification of two independent conditions on the diffusion field to seek unique solution.

Figure 4. Model of the chamber as a semi-infinite solid

Consider the chamber walls to be a semi-infinite medium as shown in Figure 4 which extend in the \(z\) direction from \(z = 0\) to \(z = \infty\). For the region \(z \geq 0\) eqn. (12)
applies. At time $t < 0$, the concentration is $C_0$ for $z \geq 0$. At $t = 0$ the surface of the semi-infinite medium ($z = 0$) the concentration $C_s > C_0$ and held there for $t > 0$. Therefore diffusion into the medium occurs.

Because eqn. (12) has one boundary (initial) condition in time and two boundary conditions in distance and is linear in the dependent variable, $C_A$, an exact solution can be obtained. Either the method of combination of variables or the Laplace transform method [Bird and Steward, 1960] is applicable. The solution was obtained using the Laplace transform method, by multiplying both sides of the eqn. (12) by $e^{-pt}$ and integrating.

\[
\int_0^\infty e^{-pt} D_{AB} \frac{\partial^2 C_A}{\partial z^2} = \int_0^\infty e^{-pt} \frac{\partial C_A}{\partial t} \tag{13}
\]

The result in terms of the fractional concentration change accomplished is:

\[
\frac{C_A - C_{As}}{C_{As} - C_{Ao}} = erfc\left(\frac{z}{\sqrt{2D_{AB}t}}\right) \tag{14}
\]

Where the complementary error function is defined as:

\[
erfc(z) = 1 - erf(x) = 1 - \frac{1}{\sqrt{\pi}} \int_0^z e^{-\eta^2} d\eta \tag{15}
\]

This equation is used to compute the concentration in the semi-infinite medium, as a function of time and distance from the surface, assuming no bulk flow. Thus, it
applies most rigorously to diffusion in solids, and also to stagnant liquids and gases when the medium is dilute in the diffusing solute.

The instantaneous rate of mass transfer across the surface of the medium \( z = 0 \) can be obtained by applying Fick's first law at the surface of the medium, see equ. 10.

Thus, referring to eqn. (13):

\[
\frac{\partial C_a}{\partial z} = \left( c_{a_0} - c_{a_z} \right) \frac{2}{\sqrt{\pi}} \exp \left( -\frac{z^2}{4D_{as}t} \right) \frac{\partial}{\partial z} \left( \frac{z}{2\sqrt{D_{as}t}} \right)
\]  

(16)

\[
\frac{\partial c_a}{\partial z} = \left( c_{a_0} - c_{a_z} \right) \frac{2}{\sqrt{\pi D_{as}t}} \exp \left( -\frac{z^2}{4D_{as}t} \right)
\]  

(17)

Substituting into Fick's first law for \( z = 0 \) the resulting equation is:

\[
n_{a_{w0}} = \frac{D_{as}}{\pi t} A (c_{a_0} - c_{a_z})
\]  

(18)

For the calculation of the mass transfer from the chamber walls eqn. (18) has been applied. Since it is assumed that atoms of naphthalene are not present in the chamber air before the burn process:

\[
n_a = \frac{D_{as}}{\pi t} A C_{naph}
\]  

(19)

Where \( t \) is the time (sec), \( A \) is the area, \( C_{naph} \) is the concentration of naphthalene and \( D_{as} \) is the diffusion coefficient of naphthalene into the air.
We can also determine the total number of moles of naphthalene \( N_A \), evaporated from the wall by integrating eqn. (19) with respect of time:

\[
N_A = \int_0^t n_{A|x=0} dt = \int_0^t \sqrt{\frac{D_{AB}}{\pi}} A \left( c_{A_i} - c_{A_0} \right) dt
\]  

(20)

\[
N_A = 2A(c_{A_i} - c_{A_0}) \sqrt{\frac{D_{AB}t}{\pi}} \quad \text{or} \quad N_A = 2Ac_{naph} \sqrt{\frac{D_{AB}t}{\pi}}
\]  

(21)

For the calculations of the instantaneous rate of mass transfer and accumulated evaporation in the function of time, a computer program was written. This is shown in the Appendix II. Results and discussion are presented in the followed chapter.

Heat Transfer Analysis

In the following analytical and numerical study, the temperature effects that result from the contained burn of solid explosive were explored. The primary focus was the prediction of the peak temperature of the gas inside an underground containment chamber as a function of the explosive consumed and the prediction of the wall surface temperature as a function of time. Parametric studies were performed using the model developed to help understand the influences of the convection heat transfer coefficient and
the thermal conductivity, density, and specific heat of the containment chamber walls.

Comparisons were made to three sets of experimental data obtained from a 1999 test series that took place at the X-Tunnel Complex at the Nevada Test Site.

Mathematical Formulation

The heat transfer between the hot combustion gases and the surface of the chamber walls is assumed to occur only by convection. Convection is further assumed to be fully established at the completion of the burn process at which time the peak temperature of the gas has been reached.

The mathematical formulation was developed in two major sections: Prediction of the Peak Gas Temperature and Prediction of the Heat Transfer to the Chamber Walls. This follows quite closely the development by Politano [1999].

The thermodynamic lumped approximation analysis is based upon a uniform-state, uniform-flow model. The principles of conservation of mass and conservation of energy were applied. The following assumptions were made: (1) the containment chamber is the control volume, (2) the combustion of the propellant adds mass to the control volume, (3) the containment chamber walls are adiabatic, (4) kinetic and potential energy effects are negligible,
(5) the initial and final states of the gas within the containment chamber are equilibrium states, and (6) the gas is assumed to be air as an ideal gas with variable specific heat.

A mass rate balance on the control volume takes the form:

\[ \Delta m_{cv} = m_p \quad \text{or} \quad m_2 = m_1 + m_p \quad (22) \]

where, \( m_p \) is the known mass of the explosive combusted, \( m_1 \) is the mass of the gas initially in the chamber, and \( m_2 \) is the total mass of the gas in the chamber after the burn process is complete. In equation (23), the mass \( m_1 \) is calculated as the density of air (at ambient temperature) multiplied by the total volume of the chamber, as calculated in Appendix I.

\[ m_1 = \rho \times V = (1.2 \frac{kg}{m^3}) \times (4644 m^3) \quad (23) \]

An energy rate balance on the control volume is:

\[ \Delta E_{cv} = Q_{cv} = W_{cv} + m_p(h_p + KE + PE) \quad (24) \]

Based on the assumptions listed above, eqn. (22) and (24) reduce to the following form of the First Law:

\[ Q_{gen} + m_p h_p = m_2 u_2 - m_1 u_1 \quad (25) \]
\( Q_{gen} \) is the total energy generated inside the containment chamber as a result of the explosive consumed. This is calculated based upon the known heat of combustion of the explosive, \( H \).

\[
Q_{gen} = H \left( \frac{\text{cal}}{\text{gm}} \right) \times \left( \frac{1000 \text{gm}}{\text{kg}} \right) \times \left( \frac{4.1868 \text{J}}{\text{cal}} \right) \times m_e(\text{kg}) \quad (26)
\]

The enthalpy of the combustion gases, \( h_p \), is based upon the known flame temperature of the propellant. The internal energy, \( u_i \), is based upon the ambient gas temperature in the chamber. Both of the above values were extracted from a table of the properties of air at low pressures [Irvine and Hartnett, 1976].

![Figure 5. The variation of internal energy with temperature for air at low pressures [Irvine and Hartnett, 1976]]
In Figure 5 only values for the temperature range of interest are presented. For the same temperature range (300-500 K) linear dependence between temperature and internal energy is assumed. The internal energy $u_i$ was solved for in eqn. (25) and the corresponding temperature $T_{\text{max}}$ was extracted from a table of the properties of air at low pressures [Irvine and Hartnett, 1976]. $T_{\text{max}}$ is assumed to be the peak temperature of the gas in the chamber after the burn process is complete.

Using the thermodynamic properties of air the peak temperature of the tunnel air following the combustion processes was found. This temperature is assumed to be the equivalent averaged value throughout the tunnel.

Once the maximum gas temperature has been established in the tunnel, we focus on the heat transfer to the wall. This will allow the wall temperature variation to be estimated.

For this analysis, time ($t = 0$) begins at the completion of the burn process, which was experimentally reported to last approximately 20 seconds [Watkins, 1999].

Considering Newton's law of Cooling:

$$\dot{Q}(t) = hA(T_a(t) - T_w(t)) \quad (27)$$
The peak temperature $T_{\text{max}}$ is substituted into eqn (27) as the initial value for $T_a(t)$ and the convection heat transfer coefficient, $h$, is taken as $36 \frac{W}{m^2 K}$. This value falls in the medium to upper range of typical values for free convection of gases [Incropera and DeWitt, 1996]. Further discussion of the influence of the convection heat transfer coefficient is provided in Chapter III. $A$ is the surface area of the chamber walls, as calculated in Appendix I. The wall surface temperature $T_w(t)$ initially taken as an ambient temperature of 295 K [Watkins, 1999]. $\dot{Q}(t)$ is solved in eqn. (27) as the maximum amount of heat that could theoretically be transferred to the chamber walls by convection.

Using the assumption that the wall is flat locally and semi-infinite, the wall surface temperature is estimated from the heat conduction solution and Duhamel's integral [Carslaw and Jaeger, 1959]:

$$T_{\text{wall}}(t) - T_{\text{wall}}(t = 0) = \frac{\alpha^{1/2}}{k_{\text{wall}} \pi^{1/2}} \int_0^t \frac{\dot{Q}(t - \tau)}{A} \frac{d\tau}{\tau^{1/2}}$$

(28)
Finally, the variation of gas temperature as a result of this heat transfer can be found from a simplified form of the First Law of Thermodynamics. This is shown in equation (29).

\[
-Q(t) = (m_c) \frac{\Delta u_{\text{gas}}}{\Delta t}
\]  

(29)

where,

\[
\Delta u_{\text{gas}} = u_z(T_{a2}) - u_z(T_{a1})
\]  

(30)

The heat transferred, \(\dot{Q}(t)\) from eqn. (27) is found for each time step and substituted into eqn. (29) to find the unknown \(u_z(T_{a2})\). Data from Figure 5 produces a new gas temperature \(T_a(t)\) at each time step. In eqn. (29) \(u_z(T_{a2})\) is the new value and \(u_z(T_{a1})\) is the previous value of the internal energy.

Eqn. (28) assumes that the containment chamber is a semi-infinite solid and that the heat flux at \(z = 0\) is a prescribed function of time, see figure 4. While this equation assumes a boundary condition of the second kind (specified heat flux), this problem actually involves a boundary condition of the third kind (convective heat transfer). A boundary condition of the second kind is, however, valid because of the numerical approach used for the solution where the heat flux is known at each time step.
The value $\dot{Q}(t - \tau)$ in eqn. (28) was taken outside the integral and held constant for each time step. This allowed eqn. (28) to be solved as a definite integral as shown in equation (31).

$$\int_{a}^{b} r^{-\frac{1}{2}} dr = 2\sqrt{b} - 2\sqrt{a} \quad (31)$$

Eqn. (28) can then be rewritten as equation (32) with the constant $c = \frac{a^{\frac{1}{2}}}{A_{K_{wall}}^{\frac{1}{2}}}$.

$$T_{wall}(t) - T_{wall}(t = 0) = c \dot{Q}(\Delta \tau) \int_{0}^{t} r^{-\frac{1}{2}} dr \quad (32)$$

Eqn. (32) was solved in discrete time intervals of $\Delta \tau$. The first three iterations are shown in equations (33), (34), and (35).

At the first time step, $t = \Delta \tau$ and the right hand side of eqn. (32) reduces to:

$$\dot{Q}(0) \times c \times (2\sqrt{\Delta \tau} - 2\sqrt{0}) \quad (33)$$

At the second time step, $t = 2\Delta \tau$ and the right hand side of eqn. (32) becomes:

$$\dot{Q}(0) \times c \times (2\sqrt{2\Delta \tau} - 2\sqrt{\Delta \tau}) + \dot{Q}(\Delta \tau) \times c \times (2\sqrt{\Delta \tau} - 2\sqrt{0}) \quad (34)$$

At the third time step, $t = 3\Delta \tau$ and the right hand side of eqn. (32) becomes:
\begin{equation}
\dot{Q}(0) \times c \times (2\sqrt{3} \Delta t - 2\sqrt{2} \Delta t) + \dot{Q}(\Delta t) \times c \times (2\sqrt{2} \Delta t - 2\sqrt{1} \Delta t) + \\
\dot{Q}(2\Delta t) \times c \times (2\sqrt{1} \Delta t - 2\sqrt{0})
\end{equation}

\dot{Q}(0) \text{ is from eqn. (27) at time } t=0, \dot{Q}(\Delta t) \text{ is from eqn. (27) evaluated at the first time step } t = \Delta t, \dot{Q}(2\Delta t) \text{ is from eqn. (27) evaluated at the second time step } t = 2\Delta t, \text{ etc. As the solution moves out in time, the right hand side of eqn. (32) approaches zero. The left hand side of eqn. (32), the wall surface temperature, starts at ambient, rises to a peak and then gradually falls back toward ambient.}

Selection of Parametric Properties

For the solution of the eqn. (28) the thermal conductivity was initially chosen as \( k = 0.81 \frac{W}{mK} \) which is a value for concrete extracted from a table of the thermo-physical properties of non-metals [Kakac and Yener, 1993]. The thermal diffusivity, \( \alpha \), was solved for as:

\begin{equation}
\alpha = \frac{k}{\rho c_p} = 4.3 \times 10^{-7} \frac{m^2}{sec}
\end{equation}
The values of density, \( \rho \), and specific heat, \( c_p \), were initially chosen as \( 2100 \, \frac{\text{kg}}{\text{m}^3} \), and \( 880 \, \frac{\text{J}}{\text{kg} \cdot \text{K}} \), respectively. These are also values for concrete extracted from a table of the thermo-physical properties of non-metals [Kakac and Yener, 1993]. Further discussion of the influence of these constants is provided in Chapter III.
CHAPTER 3

RESULTS AND DISCUSSION

Mass Transfer Results

The three sets of experimental data were considered for calculations for mass transfer analysis, and the same data were used for comparison with the results of the mathematical analysis that were performed. All three data sets were obtained from an underground test series conducted at the X-Tunnel Complex at the Nevada Test Site in 1999. Bechtel Nevada’s Special Measurement and Support section was responsible for measuring and recording a variety of physical parameters associated with each test [Watkins, 1999]. The event chamber environmental measurements include temperature measurements from an array of K-type thermocouples located in the test chamber (vertical temperature profile array), dynamic pressure, static pressure, humidity and humidity associated temperature. Three events were conducted under the code names BLACKBEARD, LAFITTE and JOLLY ROGER.

27
Figure 6. The experimental temperature variation at the wall surface for the three tests [Watkins, 1999].
The gas temperature was measured as a function of height and time in the test chamber by seven or eight thermocouples in each test. Schematics of the equipment and the chamber are shown in the Appendix I.

The figures and discussion that follow are the results of the mathematical formulation of the mass transfer from the containment chamber walls. Figure 6 shows the experimentally measured results of the wall surface temperature $T_w$ for three cases.

For prediction of the instantaneous rate of mass flow eqn. (6) and (19) are used. The solution to the model was carried out for a time period of 1800 seconds.

The results of the calculations are presented in Figures 7, 8, and 9 for the three tests: BLACKBEARD, LAFITTE and JOLLY ROGER.

In all three cases the first 1000 seconds are shown for the experimentally obtained temperatures. As expected the mass transfer increases with increasing wall temperature. Figures 7, 8 and 9 show that the rate of evaporation reaches a maximum around 100 seconds when the peak wall temperature has been reached.
Figure 7. The instantaneous rate of evaporation for naphthalene as a function of time is shown. The time-varying surface temperature measured during the Blackbeard test has been used in the calculations.
Figure 8. The instantaneous rate of evaporation for naphthalene as a function of time is shown. The time-varying surface temperature measured during the LaFitte test has been used in the calculations.
Figure 9. The instantaneous rate of evaporation for naphthalene as a function of time is shown. The time-varying surface temperature measured during the Jolly Roger test has been used in the calculations.
As the wall temperature decays with the time, the mass transfer rate decreases proportionally. From the figures it can be noticed that around 500 seconds the evaporation rate becomes very small. When the wall reaches the ambient temperature, the rate of mass transfer approaches its minimum.

Using eqn. (21) the total number of moles of naphthalene evaporated are calculated. Also the measured wall temperature data from the three experiments were used for the calculations. The solution to the model was carried out for a time period of 1800 seconds.

The results of the calculations are presented in Figures 10, 11, and 12 for the corresponding situations shown in Figures 7, 8 and 9.

Results of the mathematical model for the first 1500 seconds are shown in Figures 10, 11, 12. From the figures it can be noted that the evaporation rate rapidly increases in the first 200 seconds. It can be seen in figures 10, 11, 12, that the evaporation rate reaches almost constant values after 500 seconds.

Experimental data of the amount of evaporation during the tests was unavailable, though all three data sets are in the expected range of values.
Figure 10. The accumulated evaporation for naphthalene as a function of time is shown. The time-varying surface temperature measured during the Blackbeard test has been used in the calculations.
Figure 11. The accumulated evaporation for naphthalene as a function of time is shown. The time-varying surface temperature measured during the LaFitte test has been used in the calculations.
Figure 12. The accumulated evaporation for naphthalene as a function of time is shown. The time-varying surface temperature measured during the Jolly Roger test has been used in the calculations.
Heat Transfer Results

The system of equations, presented in the previous chapter, was solved numerically. This allowed the use of eqn. (32), which assumed a time varying heat flux for a situation that really has a time varying ambient temperature. Because an explicit-finite difference method was used, the selection of the time increment $\Delta t$ was important to the stability of the solution. In an explicit method of solution, unknown nodal temperatures for the new time are determined exclusively by the known nodal temperatures at the previous time. The initial temperature was known at time $(t = 0)$ and the calculations began at $t = \Delta t$.

The time increments were selected with a consideration for the time period of interest. Small time increments were chosen for the same time period, which was used for the three experiments conducted in X-Tunnel.

Results were found for a variety of values of the parameters to see which influenced the variation the most. Properties approximating those of concrete were used for representing the values for the wall.

Each of the tests had the identical amount of explosive weight as listed in the Table 1 [Watkins, 1999].
Table 1. Amount of propellant used in the three tests.

<table>
<thead>
<tr>
<th>Component</th>
<th>Explosive</th>
<th>Weight (pounds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>155mm shell (24 ea.)</td>
<td>Comp &quot;B&quot;</td>
<td>376.8000</td>
</tr>
<tr>
<td></td>
<td>(15.71lb/shell)</td>
<td></td>
</tr>
<tr>
<td>M112 block (48 ea.)</td>
<td>Comp C4</td>
<td>60.0000</td>
</tr>
<tr>
<td></td>
<td>(RDX)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(1.251lb./block)</td>
<td></td>
</tr>
<tr>
<td>Slip On Boosters (24 ea.)</td>
<td>PETN</td>
<td>1.0582</td>
</tr>
<tr>
<td></td>
<td>(20gram/booster)</td>
<td></td>
</tr>
<tr>
<td>Primacord (34 feet)</td>
<td>PETN</td>
<td>0.2428</td>
</tr>
<tr>
<td></td>
<td>(50 grain/foot)</td>
<td></td>
</tr>
<tr>
<td>CLSC (5 feet)</td>
<td>RDX</td>
<td>0.4285</td>
</tr>
<tr>
<td></td>
<td>(600 grain/foot)</td>
<td></td>
</tr>
<tr>
<td>RP1 Detonator (2 ea.)</td>
<td>RDX</td>
<td>0.0028</td>
</tr>
<tr>
<td></td>
<td>(0.626gram/unit)</td>
<td></td>
</tr>
<tr>
<td>RP83 Detonator (4 ea.)</td>
<td>RDX</td>
<td>0.0098</td>
</tr>
<tr>
<td></td>
<td>(1.111gram/unit)</td>
<td></td>
</tr>
<tr>
<td>Bulk C4</td>
<td>Comp C4</td>
<td>0.4286</td>
</tr>
<tr>
<td></td>
<td>(RDX)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>438.9707</td>
</tr>
<tr>
<td></td>
<td>Total Explosive Weight</td>
<td>(119.11kg)</td>
</tr>
</tbody>
</table>

The three cases were analyzed in the preliminary work to assess the effects of the combustible charge. Energy of combustion of TNT is 3579.8 cal/g, RDX 2259.2 cal/g [Watkins, 1999]. That covers the vast majority of energetic material present in tests. Comp B is 63% RDX, 36% TNT, 1% wax.

The properties of the propellant used in the analysis shown here are given in Table 2.

Table 2. Explosive Characteristics [Watkins, 1999]

<table>
<thead>
<tr>
<th>Propellant (kg)</th>
<th>Heat of Combustion (cal/gm)</th>
<th>Total Energy Generated (J)</th>
<th>Peak Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>199.115</td>
<td>2712.024</td>
<td>2.26 x 10^7</td>
<td>915.373</td>
</tr>
</tbody>
</table>
Table 2 is a summary of the propellant characteristics that are important to this study. Total energy generated is calculated in eqn. (26). Eqn. (27), (28), and (29) were solved simultaneously in an algorithm written in Java, see Appendix II. Using the data of the conducted tests and properties of the explosive used, the peak gas temperature was obtained from the eqn (25) and (26). The table of properties of air [Irvine and Hartnett, 1976] gives the value of the peak gas temperature $T_{\text{max}} = 915$ K.

Chamber Gas Temperature

The solution to the mathematical model was carried out in the time increments of $\Delta t = 10$ seconds for a time period of 1800 seconds. Results from the first 1000 iterations are shown in Figure 13. Note that time ($t=0$) starts at the completion of the burn process when the peak gas temperature has been reached. The convection heat transfer coefficient was varied from $26-46 \frac{W}{m^2K}$.

In Figure 13, the gas temperature decay with time and the influence of the heat transfer coefficient are shown.

In the Figure 13 the intermediate curve uses the previously chosen value shown in Chapter II. The other two curves represent the values for 30% lower/higher values for
heat transfer coefficient. For the values of $h$ 30% higher the gas temperature falls off more quickly compared to the originally chosen values. This value of $h$ gives the gas temperature about 15 K lower values at around 200 seconds. The values of $h$ 30% lower give the gas temperature about 30 K higher values at around 200 seconds.

Although experimental data of the wall surface temperature was unavailable for comparison, variations in the convection heat transfer coefficient from 26-46 $\frac{W}{m^2K}$ are shown. The values of the thermal diffusivity $\alpha$ is held constant at the value stated in Chapter II.

Figure 13. Calculated (predicted) gas temperature data. Effects of variations in the heat transfer coefficient are shown.
Chamber wall surface temperatures

In the Figure 13 chamber gas temperature is shown after the combustion of the explosive. The figures and discussion that follow are the results of the mathematical formulation of the heat transfer from the hot combustion gases to the containment chamber walls. Figure 14 shows the results of the gas temperature $T_g$ and the wall surface temperature $T_{wall}$ for the mathematical formulation. The solution to the model was carried out in time increments of $\Delta t = 10$ seconds for a time period of 1800 seconds. The first 1000 seconds are shown. The thermal conductivity, density, and specific heat are held constant at the values stated in Chapter II.

Figure 14 shows that the gas temperature falls off more quickly with the higher convection coefficient value but only a slight increase in the wall surface temperature is seen within the first 500 seconds. The changes in the wall temperatures happen within the first 150 seconds. It is hypothesized that a convection coefficient of $h = 36 \frac{W}{m^2K}$ is a probable choice based upon the comparisons of the wall temperatures with the experimental ones presented in the following graphs. It is seen that the wall surface temperature is approximately equal to the gas temperature.
Figure 14. Gas and wall surface temperature decay with time. Effects of variations in the heat transfer coefficient are shown.
after 800 seconds at which time the heat transfer to the chamber walls is almost zero.

In order to evaluate the effects of variations in the density, specific heat and thermal conductivity in the chamber walls, a variation on the effects of changes of thermal diffusivity \( \alpha = \frac{k}{\rho c_p} \) has been conducted. The results of the mathematical model are shown in Figure 15. The heat transfer coefficient in this case is held constant at \( h = 36 \frac{W}{m^2K} \).

The values shown in Figure 15 are the results of the mathematical model for different values of the thermal diffusivity \( \alpha \). These values are approximately \((+/- 30\%)\) compared to the values initially chosen. The curves for \( T_w(+30\%) \) and \( T_a(+30\%) \) in Figure 15 are obtained for higher values than those initially chosen. The values shown for the median curves are results for the initially chosen values of \( \alpha \) stated in the Chapter II. The values shown for \( T_w(-30\%) \) and \( T_a(-30\%) \) are for the lower values of the thermal diffusivity. In all the three cases mathematical model was solved for 1800 seconds having time increments of \( \Delta t = 10 \) seconds. Higher values for \( \alpha \) result in an increase

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Figure 15. Wall surface temperature decay with time. The heat transfer coefficient is held constant at $36 \frac{W}{m^2K}$.

Effects of variation of density, specific heat, and thermal conductivity (varied simultaneously +/- 30%) of the chamber walls is shown.
of the wall temperature of about 10 K for the whole time interval. Similar to previously, smaller values of $\alpha$ decrease wall temperature of around 10 K.

The following figures show the experimentally measured data from the three tests plotted against the results of the mathematical model. The model was solved for the data presented in Chapter II. The time increment is $\Delta r = 10$ and the time period is 1800 seconds.

In the Figures 16, 17, and 18 calculated chamber wall temperature is plotted against the results of the measurements from the tests conducted in the X-Tunnel. The model was solved for the values initially chosen in Chapter II. Although each of the tests exercises the identical amount of explosive weight (Table 1), a wide variation is shown in the experimental results. Each or the curves represents the average value of the wall temperatures measured by the thermocouples. Wide variations in the results from the thermocouples are also noticed. Measured results from the thermocouples for the three experiments can be seen in the Appendix III.
Figure 16. Measured and calculated wall surface temperatures for the Lafitte test are shown. The bar represents the range of experimental values shown in Appendix III.
Figure 17. Measured and calculated wall surface temperatures for the Bleckbeard test are shown. The bar represents the range of experimental values shown in Appendix III.
Figure 18. Measured and calculated wall surface temperatures for the Jolly Roger test are shown. The bar represents the range of experimental values shown in Appendix III.
In the Figure 19, predicted (calculated) wall
temperature is plotted and compared with the experimentally
obtained wall temperature averaged for all three tests.

Experimental results shown in Figure 19 are the
averaged values from the three experimental curves. Good
agreement is shown for the predicted temperatures compared
to the measured values. The large discrepancies between the
measured and calculated data seen in Figures 16, 17, and 18
could be attributed to the method by which the data was
measured and recorded. This could also occur if the energy
has to disperse within the tunnel over a period of time.
The mathematical model was developed to predict a peak
global average of the gas temperature for the entire
chamber, whereas the experimental data was recorded by
thermocouples in specific locations within the chamber.
Figure 19. Measured and calculated wall surface temperatures are shown. Averaged values of the measured surface temperature for all three tests are shown for comparison.
CHAPTER 4

CALCULATIONS BASED UPON WALL CONCENTRATION MEASUREMENTS

The final sets of calculations involve finding averaged concentrations of organics on the chamber walls. Personnel of the Harry Reid Center (HRC) at UNLV performed the measurements [Gonzales and Coates, 1999]. The purpose of the project was to determine the amounts of certain semi-volatile organic compounds (SVOC=s), in particular, polynuclear aromatic hydrocarbons (PAH=s) which were expected to be present as combustion products on the walls of the test chamber. Six samples were obtained within the test chamber itself and fourteen samples were taken from the tunnel walls. The samples were extracted, and the extracts concentrated and analyzed using the guidelines of EPA SW 846, Methods 3540C, 3630C, and 8270C, and the Varian Methods for SVOC=s and PAH=s [Gonzales and Coates, 1999]. Figure 20 shows the locations of the samples in the chamber walls.
The following compounds were quantified in the sample concentrates: acenaphthene, acenaphthylene, phenanthrene, anthracene, fluoranthene, pyrene, chrysene, 2,4,5-trichlorophenol, naphthalene, and fluorene. With the exception of 2,4,5-trichlorophenol, these compounds are polynuclear aromatic hydrocarbons, or PAHs, and are typically products of combustion. See Appendix IV. They are generally quite stable and would not be expected to decompose or otherwise be lost under the conditions of this analysis.

Measured concentrations of various Volatile Organic Compounds (VOCs) from the tunnel walls are then used to estimate the maximum concentrations in the tunnel air that could occur with complete evaporation.
Using the measurements made from the National Laboratory/NTS team (Appendix I), the total surface area and total volume inside the tunnel:

\[ V = 4644 \text{ m}^3 \]
\[ A = 1849 \text{ m}^2 \]

This volume can be used to estimate the mass of air in the chamber. We apply the ideal gas relationship to do this.

\[ PV = m_{\text{air}}RT \]
\[ m_{\text{air}} = 5600 \text{ (kg)} \]

From the several data values (Appendix IV), the mean for each component was determined. Then this averaged reading had to be associated with a distinct wall area. In our calculations related to these measurements, we assumed a sample area of approximately 100 in\(^2\). However, since only a fraction of the total sample collected was used in the measurements, the equivalent amount for the complete area was found. The measured values of concentration were then ratioed upward to determine an estimate for the total mass of each component on all of the chamber surfaces.

Finally, the concentration of each component was determined in the chamber if all was evaporated. Based upon the calculations shown in the section above, it seems apparent that there is a large propensity for evaporation.
Hence, it is assumed that all of each component on the wall will evaporate during the chamber heating associated with a given test.

In the table below, the calculated maximum concentrations are shown.
Table 3. Average concentrations of compounds in the wall surface from X-Tunnel

<table>
<thead>
<tr>
<th>Compound</th>
<th>Av. Concentrations of Compounds ($\mu g/in^3$)</th>
<th>Av. Concentrations of Compounds ($\mu g/m^3$)</th>
<th>Total Concentration ($\mu g$)</th>
<th>Total mass fraction (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acenaphthene</td>
<td>416.606</td>
<td>6457.416</td>
<td>11940000</td>
<td>0.0000021</td>
</tr>
<tr>
<td>Acenaphthylene</td>
<td>176.255</td>
<td>2731.957</td>
<td>5051000</td>
<td>0.0000903</td>
</tr>
<tr>
<td>Phenanthrene</td>
<td>354.933</td>
<td>5501.477</td>
<td>10170000</td>
<td>0.0001824</td>
</tr>
<tr>
<td>Anthracene</td>
<td>987.700</td>
<td>15169.880</td>
<td>28050000</td>
<td>0.0005024</td>
</tr>
<tr>
<td>Fluoranthenne</td>
<td>711.481</td>
<td>11027.993</td>
<td>20390000</td>
<td>0.0003647</td>
</tr>
<tr>
<td>Pyrene</td>
<td>1057.828</td>
<td>16396.376</td>
<td>30320000</td>
<td>0.0005417</td>
</tr>
<tr>
<td>Chrysene</td>
<td>1386.933</td>
<td>21497.457</td>
<td>39800000</td>
<td>0.0007116</td>
</tr>
<tr>
<td>2,4,5-Trichlorophenol</td>
<td>1128.050</td>
<td>17484.809</td>
<td>32330000</td>
<td>0.0005775</td>
</tr>
<tr>
<td>Fluorene</td>
<td>334.033</td>
<td>5177.521</td>
<td>9573000</td>
<td>0.0001711</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>71.680</td>
<td>1111.042</td>
<td>2054000</td>
<td>0.0000367</td>
</tr>
</tbody>
</table>
CHAPTER 5

CONCLUSION

An analysis has been performed of the possibility of evaporating an organic substance condensed on the X-tunnel walls due to heat liberated during a burn episode. The primary focus of this study was the prediction of the amount of evaporation for different types of organic materials from the underground containment chamber as a function of time. A mathematical model has successfully been developed that gives a reasonable approximation of the rate of evaporation and offers an estimate of the amount of evaporation variations with time.

It is shown that there is a high probability that a rapid evaporation process could take place. From this work, it is concluded that virtually any amount of most typical semivolatile organic would be evaporated from the wall as the result of the temperature transients typically experienced.

To study mass transport from the semi-infinite media, prediction of wall and ambient temperature were made as a
function of time. Satisfactory results are shown for the predicted temperature compared to the measured values. Parametric studies that were performed with the model provided some insights as to the influences of the convection heat transfer coefficient, thermal conductivity, density, and specific heat of the containment chamber walls. Although wide variations from the experimentally measured temperatures can be noticed, averaged values from the three tests give good agreement with the results of the model.

Additionally, estimates of maximum concentrations of evaporated materials in the tunnel air (from previously measured concentrations in the tunnel walls) are performed. It appears that the contribution of tunnel surface archives to the overall amount of semivolatiles will be quite small.

Satisfactory results were obtained that will aid in the engineering design of containment chambers for future contained burn processes involving different types and amounts of propellant. The properties of the propellant that are necessary to carry out the solution are the mass, heat of combustion, and the flame temperature. The physical attributes of the containment chamber such as the volume surface area of the walls, and thermo-physical properties can be varied with relative ease.
APPENDIX I

SCHEMATICS OF THE EQUIPMENT AND DIMENSIONS OF THE CHAMBER

Schematics of the equipment for wall temperature measurements [Watkins, 1999]:

Figure 21. Thermocouple information data
THERMOCOUPLE ARRAY ELEMENTS: 1TC @ -2' FROM BACK, 2TC @ -7' FROM BACK, 3TC @ -12 FROM BACK, 4TC @ -17 FROM BACK, 5TC @ -22 FROM BACK, 6TC @ -27 FROM BACK, 7TC @ -32 FROM BACK. (APPROX. FIVE FOOT CENTERS AND TWO FEET FROM INVERT AND BACK)

ELEMENTS 1TC, 4TC AND 7TC HAVE GAS SAMPLE TUBES NEXT TO THEM AS SHOWN ABOVE.

THERMOCOUPLE SUPPORT
NO SCALE

THERMOCOUPLE WRAPPED IN HIGH TEMPERATURE INSULATION TO BREAK BEAM HEAT SINK PATH AND DAMP TRANSDUCER VIBRATION, SHOWN CLIPPED TO SUPPORT STRUCTURE

THRUWIRE THERMOCOUPLE ARRAY ELEMENTS: 1TC @ -2' FROM BACK, 2TC @ -7' FROM BACK, 3TC @ -12 FROM BACK, 4TC @ -17 FROM BACK, 5TC @ -22 FROM BACK, 6TC @ -27 FROM BACK, 7TC @ -32 FROM BACK. (APPROX. FIVE FOOT CENTERS AND TWO FEET FROM INVERT AND BACK)

ELEMENTS 1TC, 4TC AND 7TC HAVE GAS SAMPLE TUBES NEXT TO THEM AS SHOWN ABOVE.
<table>
<thead>
<tr>
<th>Mnemonics</th>
<th>Transducer</th>
<th>Station/Channel</th>
<th>Location</th>
<th>Type</th>
<th>Serial #</th>
<th>Range</th>
<th>Operate Range</th>
<th>System Range</th>
<th>Full Scale Voltage</th>
<th>Cal Step (Volts)</th>
<th>Recording Mers Rate</th>
<th>Filt Num Jets</th>
<th>Smalls Slot Chan</th>
</tr>
</thead>
<tbody>
<tr>
<td>TC1</td>
<td>SHEATHED</td>
<td>TC1 TOP</td>
<td>~3' (2' FROM BACK)</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>2K</td>
<td>1</td>
</tr>
<tr>
<td>TC2</td>
<td>SHEATHED</td>
<td>TC2 CAVITY LEFT</td>
<td>~27' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>2K</td>
<td>2</td>
</tr>
<tr>
<td>TC3</td>
<td>SHEATHED</td>
<td>TC3 BEAM</td>
<td>~22' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>3K</td>
<td>3</td>
</tr>
<tr>
<td>TC4</td>
<td>SHEATHED</td>
<td>TC4 BEAM</td>
<td>~17' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>4K</td>
<td>4</td>
</tr>
<tr>
<td>TC5</td>
<td>SHEATHED</td>
<td>TC5 CHAMBER TDL BOX</td>
<td>~16' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>5K</td>
<td>5</td>
</tr>
<tr>
<td>TC6</td>
<td>SHEATHED</td>
<td>TC6 SHOTCRETE</td>
<td>~12' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>6K</td>
<td>6</td>
</tr>
<tr>
<td>TC7</td>
<td>SHEATHED</td>
<td>TC7 BEAM</td>
<td>~12' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>7K</td>
<td>7</td>
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<tr>
<td>TC8</td>
<td>SHEATHED</td>
<td>TC8 BEAM</td>
<td>~7' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>8K</td>
<td>8</td>
</tr>
<tr>
<td>TC9</td>
<td>SHEATHED</td>
<td>TC9 BEAM</td>
<td>~2' FROM INVERT</td>
<td>Tj36-Cain-316U</td>
<td>NONE</td>
<td>1250C</td>
<td>240C</td>
<td>300C</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>9K</td>
<td>9</td>
</tr>
</tbody>
</table>

NOTE: TC'S ARE CUSTOM MADE OMEGA TYPE K THERMOCOUPLES - EXTENSION # AFTER 316U IS LENGTH IN INCHES

| PX10      | SHAFT NEAR BARRIER LEFT RIB J BOX | SMI 601338-4 | 500 PSIA | 80 PSIA | 100 PSIA | 5 | 1 | 4 | 10 | 2K | 10 | 500 | 1 | 1 | 2 | 1 |
| PX11      | SHAFT NEAR BARRIER LEFT RIB J BOX | SMI 601338-4 | 500 PSIA | 80 PSIA | 100 PSIA | 5 | 1 | 4 | 11 | 2K | 11 | 500 | 2 | 2 | 2 | 2 |
Figure 22. Dimensions of the chamber:

Total surface area (half cylinder + floor + ends):

\[ S = \frac{2\pi rL}{2} + 2rL + 2\left(\frac{\pi r^2}{2}\right) = 1849(m^2) \]

Total chamber volume:

\[ V = \frac{\pi r^2 h}{2} = 4644(m^3) \]
APPENDIX II

COMPUTER CODES

Mass transfer calculations

```c
#include <stdlib.h>
#include <fstream.h>
#include <iostream.h>
#include <strstream.h>
#include <stdlib.h>
#include <vector>
#include <cmath>
#include <string>

#define PI 3.14

vector<long double> na_results;

double Pi(double T, int t)
{
    double result;
    double A1 = 34.9161;
    double B1 = -3935.7;
    double C1 = -9.0648;
    double D1 = -2.0672;
    double E1 = 1.5550*0.000001;
    double CON = 133.322368;
    double expnt =
        A1 + B1/T + C1*log10(T) + D1*T*0.000000001 + E1*T*T;

    cout << "Exponent in PI: " << expnt << endl;
    result = CON*pow(10, expnt);
    cout << "Pi(T): " << result << endl;
    return result;
}
```

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double Con (double T, int t) {
    double result;
    double CON1 = 0.0000098692;
    double Rg = 0.08205/1000;
    result = (PI(T,t)*CON1)/(Rg*T);
    cout << "Con(T): " << result << endl;
    return result;
}

double D12(double T, int t) {
    double result = 0.00000706*(pow((T/298.15),1.75));
    cout << "D12(T): " << result << endl;
    return result;
}

long double na(double T, int t) {
    long double result;
    double d12;
    int A = 1;
    d12 = D12(T, t);
    result = sqrt(d12/(PI*t)) * A * Con(T, t);
    cout << "na(T): " << result << endl;
    return result;
}

double NA(double T, int t) {
}

long double NAReal(double T, int t) {
    double A = 1;
    double result;
    result = 2*A*Con(T,t)*sqrt((D12(T,t)*t)/PI);
    cout << "NA(T): " << result << endl;
    return result;
}

void func1(char* infname, int t, bool incr) {
    ifstream infile;
    ofstream nafile, NAfile1, NAfile2;
cout << "in " << infname << endl;
infile.open(infname);
if (!infile.good()) {
    cout << "I can not open the file " << infname << endl;
    return;
}
string nafname = "na";
string NAfname1 = "NAAdd";
string NAfname2 = "NAForm";
if (incr) {
    nafname += string("_1\0");
    NAfname1 += string("_1\0");
    NAfname2 += string("_1\0");
}
nafname += string(".txt\0");
NAfname1 += string(".txt\0");
NAfname2 += string(".txt\0");
nafile.open(nafname.c_str());
if (!nafile.good()) {
    cout << "I can not open the file " << nafname << endl;
infile.close();
return;
}
NAfile1.open(NAfname1.c_str());
if (!NAfile1.good()) {
    cout << "I can not open the file " << NAfname1 << endl;
infile.close();
nafile.close();
return;
}
NAfile2.open(NAfname2.c_str());
if (!NAfile1.good()) {
    cout << "I can not open the file " << NAfname2 << endl;
infile.close();
nafile.close();
NAfile1.close();
return;
}

double T;
while (infile>>T) {
cout << \nT = " << T << " t = " << t << endl;
long double na_val = na(T,t);
long double NAValReal = NAReal(T,t);
na_results.push_back(na_val);
naf ile << na_val << endl;
NAfile2 << NAvalReal << endl;
if (incr)
    t++;}
// calculation of NA from results
// from na to vector na_results
long double NAval = 0;
int i;
for (int i = 0; i < na_results.size(); i++) {
    NAval = NAval + na_results[i];
    NAfile1 << NAval << endl;
} infile.close();
naf ile.close();
NAfile1.close();
NAfile2.close();
}

// usage: a.out <infile> t Y/N
int main(int argc, char* argv[])
{
    // argv[3] - increment (Y/N)
    bool incr = false;
    char* tval = argv[2];
    int t = atoi(tval);
    char* str = argv[3];
    if (!strcmp(str, "Y"))
        incr = true;
    funct(argv[1], t, incr);
    return 1;
}
Wall And Ambient Temperature Calculations

```java
import java.ic.*;
import java.awt.*;
import java.applet.Applet;
import java.awt.event.*;

public class calculateTWall extends Applet implements ActionListener
{
    int SOne, Ee, IOne, data_count;
    double twall, Ma, Ta, U;
    // vo calculateFun() double X[][] = 0;
    double k, asv;
    String filename, filename2;

    Label label1, label2, label3, label4, label5, label6;
    Label hminLB, hmaxLB, stepLB, alphaLB, resultLB;
    TextField text1, text2, text3, text4, text5, text6;
    TextField hminTXT, hmaxTXT, stepTXT, alphaTXT;
    Button calculate;
    DataOutputStream outFile, outFile1;

    public void init()
    {
        // creation and initialization
        label1 = new Label("Enter T a (0) gas temperature");
        label2 = new Label("Enter Ee duration");
        label3 = new Label("Enter IOne time increment");
        label4 = new Label("Enter U internal energy");
        label5 = new Label("Enter Ma (mass of the propelant+gas)");
        label6 = new Label("Enter filename for results");
        hminLB = new Label("Hmin");
        hmaxLB = new Label("Hmax");
        stepLB = new Label("Step");
        alphaLB = new Label("Alpha");
        resultLB = new Label("Start");

        text1 = new TextField(15);
        text2 = new TextField(15);
        text3 = new TextField(15);
        text4 = new TextField(15);
        text5 = new TextField(15);
        text6 = new TextField(15);
    }
}
```

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text6 = new TextField(50);
hminTXT = new TextField(5);
hmaxTXT = new TextField(5);
stepTXT = new TextField(5);
alphaTXT = new TextField(15);
calculate = new Button("Calculate");
calculate.addActionListener(this);
add(hminLB);
add(hminTXT);
add(hmaxLB);
add(hmaxTXT);
add(stepLB);
add(stepTXT);
add(alphaLB);
add(alphaTXT);
add(label1);
add(text1);
add(label2);
add(text2);
add(label3);
add(text3);
add(label4);
add(text4);
add(label5);
add(text5);
add(label6);
add(text6);
add(calculate);
add(resultLB);
k = 0.81;
asv = 1849;
}

public void actionPerformed(ActionEvent e) {
    resultLB.setText("Start calculating...");
    try {
        calculateFun();
    } catch (IOException io) {
        System.err.println("Greska !!");
    }
    resultLB.setText("Done !");
}
public void calculateFun() throws IOException
{
    double X[][];
    filename = text6.getText();
    filename2 = new String("c:\\Zoran\\probI\\ultal");
    int h1, h2, step;

    h1 = Integer.parseInt(hminTXT.getText());
    h2 = Integer.parseInt(hmaxTXT.getText());
    step = Integer.parseInt(stepTXT.getText());
    double alfa, c;
    alfa = Double.valueOf(alphaTXT.getText()).doubleValue();
    c = Math.sqrt(alfa)/(asv*k*Math.sqrt(3.1459));
    SOne = 0;
    Ma = Double.valueOf(text5.getText()).doubleValue();
    Ee = Integer.parseInt(text2.getText());
    IOne = Integer.parseInt(text3.getText());
    data_count = (Ee-SOne)/IOne;
    X = new double[data_count][data_count];
    if (data_count == 0) {
        twall = S00;
        return;
    }

    for (int h = h1; h <= h2; h+=step) {
        String filename1, filename3;
        String line;

        filename1=filename+"h"+Integer.toString(h)+"alpha"+Double.toString(alfa);

        filename3=filename+"h"+Integer.toString(h)+"alpha"+Double.toString(alfa);
        // output to file1, file3
        DataOutputStream outFile, outFile1;

        outFile = new DataOutputStream(new FileOutputStream(filename));
        outFile1 = new DataOutputStream(new FileOutputStream(filename3));
        // catch (IOException e) {
        // System.err.println("I can not open the fajl
        outFile = new DataOutputStream(new FileOutputStream(filename1));
        outFile1 = new DataOutputStream(new FileOutputStream(filename3));
        // catch (IOException e) {
        // System.err.println("I can not open the fajl
        outFile = new DataOutputStream(new FileOutputStream(filename1));
        outFile1 = new DataOutputStream(new FileOutputStream(filename3));
        // catch (IOException e) {
        // System.err.println("I can not open the fajl
    }

    return;
}
//
int t = S0ne;
double Tw0, Ta0, Tw;
Tw0=Tw=300;

Ta0=Ta=Double.valueOf(text4.getText()).doubleValue();
double Qw0, Qw;
Qw0 = h*asv*(Ta-Tw0);
Qw = Qw0;

for (int i = S0ne; i <= data_count; i++) {
    double U1 = (-Qw+IOne/Ma)+h;
    double Tal = (U1+3254.67)/724.589;
    // outfile
    line = Double.toString(U1)+"+
    try {
        outFilel.writeUTF(line);
    } catch (IOException io) {
        System.err.println(io.toString());
    }
    Ta = Tal;
    X[i][0] = Ta;
    X[i][3] = t;
    X[i][2] = Qw;
    AddTerm(X, i, c, h, alfa);
    // outfile
    line = Integer.toString(t)+"+
    try {
        outFile.writeUTF(line);
    } catch (IOException io) {
        System.err.println(io.toString());
    }
    Tw = twall;
    X[i][1] = twall;
    Qw = h*asv*(Ta-Tw);
    h = h1;
    t += IOne;
} // close the file
try {
    OutFilel.close();
    OutFile.close();
}
catch (IOException io) {
    System.err.println(io.toString());
}
X[0][2] = Qw0;
X[0][0] = Ta0;
} // end for h
}

public void AddTerm(double X[][], int j, double cc, int h, double alfa) {
    double one, two, ccTsub;
    double tj, tj1, tj2, Qj, Qj1, Qj2, Q0, Qm, Sq0l, Sql;
    int m, L;
    double tsub;
    Q0 = X[0][2];
    tsub = twall = 0;
    tj = X[j][2];
    if (j > data_count + 1)
        Qj2 = X[j+1][2];
    else
        Qj2 = 0;
    if (j > 0)
        Qj1 = X[j-1][2];
    else
        Qj1 = Q0;
    Sq0l = 2*Math.sqrt(IOne)-2*Math.sqrt(SOne);
    m = j;
    for (L = 1; L <= j; L++) {
        Qm = X[L-1][2];
        Sql = 2*Math.sqrt(X[m][3]) - 2*Math.sqrt(X[m-1][3]);
        tsub = tsub + Qm*Sql;
        m = m-1;
    }
    one = Math.sqrt(alfa)*tsub;
    two = asv*k*Math.sqrt(3.1459);
    ccTsub = one/two;
    twall = ccTsub+300;
}
Appendix III

MEASURED TEMPERATURES FOR THE THREE TESTS [WATKINS, 1999]

Figure 23. Variations of the measured temperatures from the thermocouples for Blackbeard test are shown.
Figure 24. Variations of the measured temperatures from the thermocouples for Lafitte test are shown.
Figure 25. Variations of the measured temperatures from the thermocouples for Jolly Roger test are shown.
APPENDIX IV

TABLES OF ELEMENTS IN THE TUNNEL WALL

Table 4. Concentrations of Compounds in Surface Samples from X-Tunnel, μg/100(in²) [Gonzales and Coates, 1999].

<table>
<thead>
<tr>
<th>COMPOUND</th>
<th>1-1</th>
<th>1-2</th>
<th>1-3</th>
<th>1-4</th>
<th>1-5</th>
<th>1-6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acenaphthene</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td>Acenaphthylene</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td>Phenanthrene</td>
<td>152.7</td>
<td>110.3</td>
<td>280.8</td>
<td>284.8</td>
<td>719.3</td>
<td>ND</td>
</tr>
<tr>
<td>Anthracene</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td>Fluoranthene</td>
<td>120.9</td>
<td>87.7</td>
<td>134.4</td>
<td>116.6</td>
<td>143.8</td>
<td>ND</td>
</tr>
<tr>
<td>Pyrene</td>
<td>113.2</td>
<td>82.6</td>
<td>121.1</td>
<td>104.9</td>
<td>169</td>
<td>ND</td>
</tr>
<tr>
<td>Chrysene</td>
<td>ND</td>
<td>ND</td>
<td>362.2</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td>2,4,5- Trichlorophenol</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td>Fluorene</td>
<td>100.0</td>
<td>64.8</td>
<td>215.9</td>
<td>238.0</td>
<td>97.5</td>
<td>ND</td>
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<tr>
<td>Naphthalene</td>
<td>70.4</td>
<td>50.4</td>
<td>104.2</td>
<td>61.6</td>
<td>71.8</td>
<td>ND</td>
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**Set II**

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<th>2-2D</th>
<th>2-3</th>
<th>2-3D</th>
<th>2-4</th>
<th>2-5</th>
<th>2-6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acenaphthene</td>
<td>1.32</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
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<td>ND</td>
</tr>
<tr>
<td>Acenaphthylene</td>
<td>1.41</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td>Phenanthrene</td>
<td>80.8</td>
<td>151.9</td>
<td>142.4</td>
<td>138.4</td>
<td>142.4</td>
<td>10.3</td>
<td>77.5</td>
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<td>Anthracene</td>
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<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
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<td>Fluoranthene</td>
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<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>3.00</td>
<td>ND</td>
<td>ND</td>
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<tr>
<td>Pyrene</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
</tr>
<tr>
<td>Chrysene</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
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<tr>
<td>2,4,5-Trichlorophenol</td>
<td>ND</td>
<td>ND</td>
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<td>ND</td>
</tr>
<tr>
<td>Fluorene</td>
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<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
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<td>ND</td>
<td>ND</td>
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<td>ND</td>
<td>ND</td>
<td>ND</td>
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</tr>
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</table>

**Set III**

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<th>3-3</th>
<th>3-3D</th>
<th>3-4</th>
<th>3-5</th>
<th>3-6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acenaphthene</td>
<td>650.6</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>598.5</td>
<td>ND</td>
</tr>
<tr>
<td>Acenaphthylene</td>
<td>351.1</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
<td>ND</td>
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VITA

Graduate College
University of Nevada, Las Vegas

Zoran Stefanoski

Home address:
444 Saratoga Ave. #28E
Santa Clara, CA, 95050

Degrees:
Bachelor of Science, Mechanical Engineering, 1996
St. Kiril & Metodij University, Skopje, Macedonia

Thesis Title: Estimation of Evaporation of Previously Condensed Hydrocarbons in a Tunnel Burn Experiment

Thesis Examination Committee:
Chairperson, Dr. Robert F. Boehm, Ph.D.
Committee Member, Dr. Zhiyong Wang, Ph.D.
Committee Member, Dr. Yi-Tung Chen, Ph.D.
Grad. Faculty Representative, Dr. Hossein Tehrani, Ph.D.