Nitrous Oxide Decomposition for Supersonic Combustion Experiments in the USQ Ludwieg Tube Facility

D.R. Buttsworth[*]

Faculty of Engineering and Surveying
University of Southern Queensland QLD 4350 Australia

Abstract

Wind tunnel facilities are required to support the development of the scramjet engine. The performance of a short duration wind tunnel which uses the thermal decomposition of nitrous oxide to augment the flow stagnation enthalpy is simulated in the present work. In its normal model of operation, the wind tunnel being considered uses a free piston compression process to compress the test gas to a moderate stagnation temperature and pressure, suitable for cold flow hypersonic aerodynamics experiments. However, by introducing a mixture of nitrous oxide and nitrogen ahead of the piston, it should be possible to provide a test gas which closely simulates the properties of air. A simulation which models the thermo-chemistry of the free piston compression process with nitrous oxide is described. Results indicate that relatively large magnitude fluctuations in the test gas are likely to arise due to the rapid decomposition process, rendering the compressed gas unsuitable for supersonic combustion testing. Piston braking or some other change to the configuration would be necessary in order to successfully use nitrous oxide decomposition to enhance the enthalpy of the test gas.

Keywords: Nitrous oxide, Thermal decomposition, Short duration wind tunnel.

1. Introduction

Scramjet engine development is likely to continue to rely on high quality wind tunnel facilities in the immediate future. Short duration wind tunnel facilities such as free piston shock tunnels can be used for scramjet experiments, and such facilities have been successfully operated in University laboratories, Stalker [1]. However, free piston shock tunnels typically have a test duration limited to a few milliseconds. For scramjet configurations with zones of subsonic or separated flow, or for dynamic experiments on thermal choking or scramjet engine starting, longer test flow durations are required.

Relatively long duration hypersonic flows which last on the order of 100 ms can be achieved using a piston to directly compress the test gas. Gun tunnels, Ludwieg tubes with isentropic compression heating, and long-shot tunnels are examples of facilities producing relatively long duration hypersonic flows. However, the stagnation enthalpy produced in such facilities is generally not sufficient for scramjet combustion experiments.

The thermal decomposition of nitrous oxide is exothermic and can be used to boost the stagnation enthalpy of wind tunnel flows. For example, some early work in the 1960s was performed by Williams [2] who described the used N_2O in a hot-shot facility, and Craig and Ortwerth [3] who describe the use of N_2O in shock tunnels. Wind tunnel investigations using N_2O either by itself or supplemented with other combustible gases have been performed over the subsequent decades in a variety of tunnel configurations [4-6].

A Ludwieg tube with free piston compression heating exists at the University of Southern Queensland. By adding nitrous oxide to the test gas which is compressed by the piston, it should be possible to augment the stagnation temperature of the test gas while retaining a test gas composition which closely resembles that of air.

The purpose of the current paper is to assess the prospects for using nitrous oxide to increase the stagnation enthalpy of an air-like test gas in order to produce conditions appropriate for supersonic combustion experiments in the USQ Ludwieg tube facility.

2. Facility Arrangement

The Ludwieg tube facility at USQ uses a free piston compression process to generate a test gas at temperatures and pressures suitable for hypersonic testing. The general arrangement of the facility is illustrated in Fig. 1. A valve initially separates the reservoir and the Ludwieg tube and when this valve is opened, the piston is driven down the tube. The test gas, which initially resides in the region ahead of the piston, is compressed by the movement of the piston. Stagnation temperatures and pressures appropriate for cold-flow hypersonic testing can be generated through the piston compression process. The primary geometric characteristics of the facility are presented in Table 1.
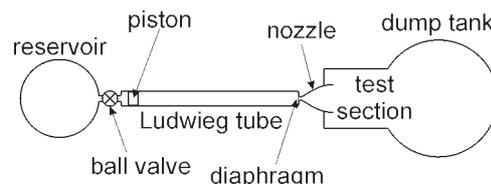

Figure 1. Schematic illustration of the Ludwieg tube facility.

---
* Corresponding author:
Phone: (+61) 7 4631 2614
Email: david.buttsworth@usq.edu.au

Table 1. Principal dimensions of Ludwieg tube for simulations.

Component	Characteristic
Reservoir	$V = 0.355$ m^3
Ball valve	$d = 28$ mm (max)
Piston	$m_p = 0.2$ kg
Barrel	$L = 16$ m; $d = 0.13$ m
Nozzle throat	$d = 28.84$ mm
Dump tank	$V = 12.7$ m^3

2. Nitrous Oxide

The thermal decomposition of nitrous oxide might be written as the global process

$$2N_2O \rightarrow 2N_2 + O_2 + \text{heat.}$$
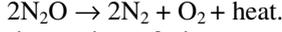
Assuming air consists of nitrogen and oxygen only with mole fractions: $x_{N2} = 0.79$, $x_{O2} = 0.21$, for complete decomposition of the nitrous oxide to yield an air-like test gas, the initial filling conditions for the Ludwieg tube should be: $x_{N2O} = 0.53$, $x_{N2} = 0.47$.

The adiabatic flame temperature for the decomposition of pure nitrous oxide is somewhat less than a typical stoichiometric hydrocarbon-air mixture, and reduces to about 1360 K for the diluted mixture required for production of the air-like test gas, Fig. 2.
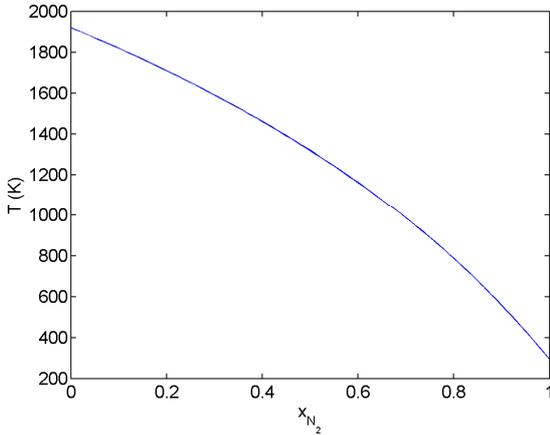

Figure 2. Constant pressure adiabatic flame temperatures for N$_2$O mixtures with different mole fractions of N$_2$ assuming complete decomposition of N$_2$O.

3. Model

3.1 Overview

The performance of the Ludwieg tube facility with thermal decomposition of the nitrous oxide is assessed using a coupled chemical and thermal model. Four different regions are treated by the model as illustrated in Fig. 3.

3.2 Thermodynamics

For region 1, treating the compressed air as a perfect gas with constant specific heats, the uniform state, uniform flow energy equation can be written

$$\dot{T}_1 = \frac{\dot{Q}_{in,1}}{m_1 c_v} + \frac{\dot{m}_1}{m_1}(\gamma - 1)T_1 \qquad (1)$$

Adopting a similar approach for region 2 and recognizing the need to incorporate the piston work, the energy equation can be written
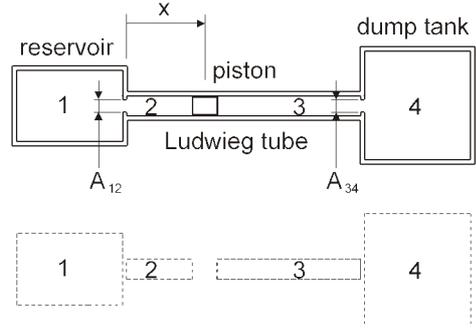

Figure 3. Illustration of the four regions used in the thermodynamic model.

$$\dot{T}_2 = \frac{\dot{Q}_{in,2}}{m_2 c_v} + \frac{\dot{m}_2}{m_2}(T_1\gamma - T_2) - \frac{p_2}{m_2 c_v}\dot{V}_2 \qquad (2)$$

When no chemical reactions occur in region 3, the energy equation can be written

$$\dot{T}_3 = \frac{\dot{Q}_{in,3}}{m_3 c_v} + \frac{\dot{m}_3}{m_3}(\gamma - 1)T_3 - \frac{p_3}{m_3 c_v}\dot{V}_3 \qquad (3)$$

which accommodates the piston work on the gas in region 3 and the possibility of discharge from the nozzle throat when the diaphragm is ruptured.

Pressure, which appears in (2) and (3), is obtained from the ideal gas law using the temperature, mass, and volume of the respective regions. The instantaneous volume in regions 2 and 3, and the volume derivatives which appear in (2) and (3), are determined from the cross sectional area of the barrel and the piston position (x) and velocity ($\dot{x}$), as discussed below.

For region 4, the energy equation is

$$\dot{T}_4 = \frac{\dot{Q}_{in,4}}{m_4 c_v} + \frac{\dot{m}_4}{m_4}(T_3\gamma - T_4) \qquad (4)$$

Indicating that there will be no change of conditions in region 4 unless there is either heat transfer or discharge through the nozzle.

The mass flow rate through the ball valve is modeled using

$$\dot{m}_2 = A_{12}\sqrt{2p_1\rho_1 \frac{\gamma}{\gamma-1}\left(\frac{p_{th}}{p_1}\right)^{\frac{2}{\gamma}}\left[1 - \left(\frac{p_{th}}{p_1}\right)^{\frac{\gamma-1}{\gamma}}\right]} \qquad (5)$$

The flow area available for discharge from the reservoir into the barrel (A_{12}) is specified as function of time to accommodate the finite opening time of the ball valve (see Section 4). The throat pressure (p_{th}) is taken as

$$p_{th} = p_1\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} \quad \text{if} \quad p_2 \leq p_1\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}}$$

$$p_{th} = p_2 \quad \text{if} \quad p_2 > p_1\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}}$$

Discharge through the nozzle throat will occur if the pressure differential across the diaphragm exceeds the designed rupture pressure. It is assumed that the diaphragm rupture is instantaneous such that the full flow area of the throat is immediately available for discharge from the Ludwieg tube into the test section. Hence another differential equation is available and the form of the model for the nozzle throat discharge ($\dot{m}_4$) is identical to that of the ball valve discharge model ($\dot{m}_2$) as given by (5).

From the conservation of mass, the mass flow rate out of regions 1 and 3 at any point in time matches the instantaneous mass flow rate into regions 2 and 4 respectively. Hence the instantaneous value of mass in regions 1 and 3 can be obtained from the integration of the equations for $\dot{m}_4$ and $\dot{m}_2$ if the initial values of m in these regions are known.

The piston velocity, which is necessary for the evaluation of the volume derivatives in (2) and (3), is obtained from Newton's law,

$$\ddot{x} = \frac{(p_2 - p_3)A_3 - F_p}{m_p} \tag{7}$$

where F_p is the friction on the piston which acts in a direction opposite to the piston velocity and which can be modeled in various ways.

The system of equations described above represents a system of coupled ODEs in the unknowns (T_1, T_2, T_3, T_4, m_2, m_4, x, $\dot{x}$) which can be solved via numerical integration for particular initial conditions.

3.3 Chemical Kinetics

For cases where decomposition of N_2O was considered, (3) was replaced by the following system of equations:

$$\dot{T}_3 = \frac{\frac{\dot{Q}_{in,3}}{V_3} - p_3\frac{\dot{V}_3}{V_3} + p_3\frac{\sum \dot{\omega}_i}{\sum[X_i]} - \sum \bar{h}_i\dot{\omega}_i + \frac{\dot{m}_3}{m_3}(p_3 + \sum[X_i]\bar{h}_i)}{\sum[X_i]\overline{C_{p_i}} - \frac{p_3}{T_3}} \tag{8}$$

$$[\dot{X}_i] = \dot{\omega}_i - [X_i]\frac{\dot{V}_3}{V_3} \tag{9}$$

where the new symbols introduced above have the following meanings: $[X_i]$ – molar concentration of species i (kmol/m^3), $\dot{\omega}_i$ – species production rate (kmol/s-m^3), $\overline{C_{p_i}}$ – constant pressure specific heat on a molar basis (J/kmol-K), $\bar{h}_i$ – enthalpy on a molar basis (J/kmol).

The set of reactions considered in the present work for representing the thermal decomposition of N_2O are presented in Table 2. The primary reactions for the decomposition of N_2O are reactions 1-3. However, reactions 4-6 have been included because without these mechanisms, the overall conversion of N_2O to N_2 and O_2 was delayed by about 100 ms at the condition considered in the present work. Reactions 7 and 8 have been included because they appear to influence the rate at which [NO] approached the equilibrium value.

Table 2. Reaction mechanism rate coefficients according to [7]. The form is $k_f = AT^\beta \exp(-E/R_u T)$ and units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	Reaction	A	β	E
1	$N_2O + M \rightarrow N_2 + O + M$	1.60e+14	0.000	51600
2	$N_2O + O \rightarrow N_2 + O_2$	1.00e+14	0.000	28200
3	$N_2O + O \rightarrow 2NO$	1.00e+14	0.000	28200
4	$NO_2 + O \rightarrow NO + O_2$	1.00e+13	0.000	600
5	$NO_2 + M \rightarrow NO + O + M$	1.10e+16	0.000	66000
6	$2O + M \rightarrow O_2 + M$	1.89e+13	0.000	-1788
7	$N + NO \rightarrow N_2 + O$	3.27e+12	0.300	0
8	$N + O_2 \rightarrow NO + O$	6.40e+09	1.000	6280

3.4 Implementation

The model was implemented in the Matlab environment. Thermodynamic polynomials were used for the calculation of the required gas properties including the equilibrium constants and reverse reaction rates. These polynomial were obtained from the GRI-Mech database. The governing equations were integrated from the initial conditions using the standard Matlab function, 'ode15s'.

4. Results

To avoid piston oscillations during the compression process it is necessary to ensure the ball valve is not opened too quickly (Jones et al. [8]). For simulations of the present conditions, this is achieved using an area variation illustrated in Fig. 4.
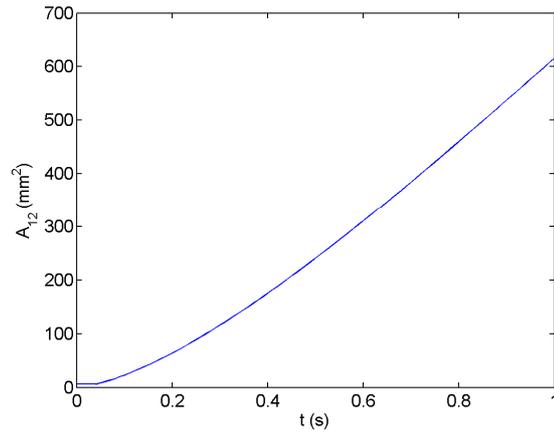

Figure 4. Profiles of valve open area as a function of time

Figures 5, 6, and 7 present results from the simulations for two cases: (1) the piston compresses an air-like mixture of N_2 and O_2; and (2) the piston compresses an appropriate mixture of N_2 and N_2O. In both cases, the initial pressure and temperature of the gas in the barrel was 100 kPa and 500 K respectively. The initial pressure and temperature of the air in the reservoir was 20 MPa and 293 K. The diaphragm bursting pressure was set sufficiently high to ensure no discharge through the nozzle for these initial simulations. Furthermore, only the adiabatic performance was simulated, and the piston was considered frictionless.
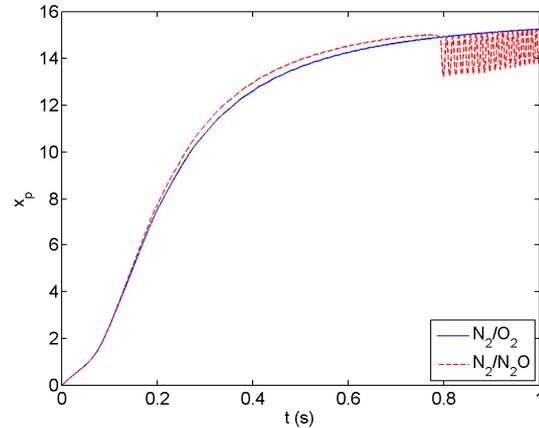

Figure 5. Piston position a function of time.

The most notable feature of the simulations is the generation of substantial fluctuations in piston position (Fig. 5), and in the gas pressure (Fig. 6) and temperature (Fig. 7) when the nitrous oxide decomposes. These oscillations arise because the piston has a finite, non-zero mass, and the gases in the tube have finite, non-zero effective stiffness. The natural frequency of the equivalent spring-mass system calculated using the mean piston position and mean pressure at about 0.9 s (Figs. 5 and 6) corresponds closely with the natural frequency of the oscillations observed in these figures.
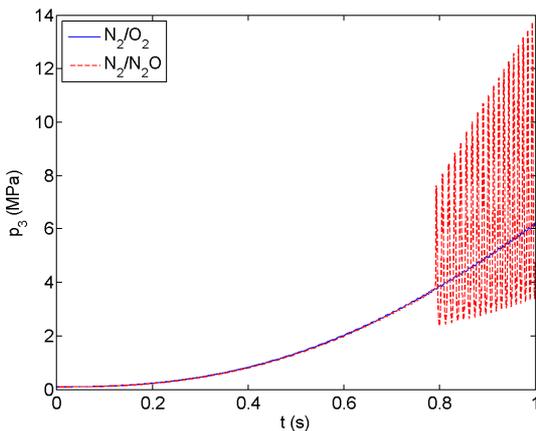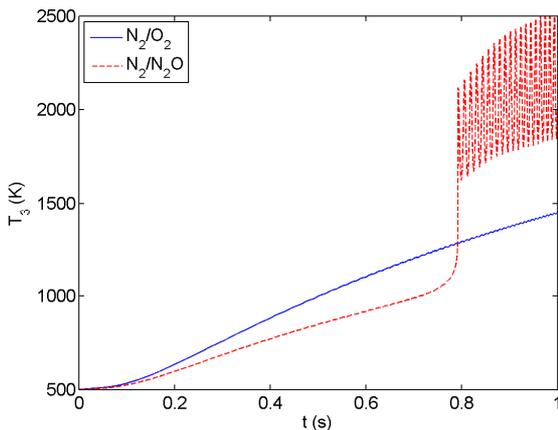

Figure 6. Barrel pressure as a function of time.

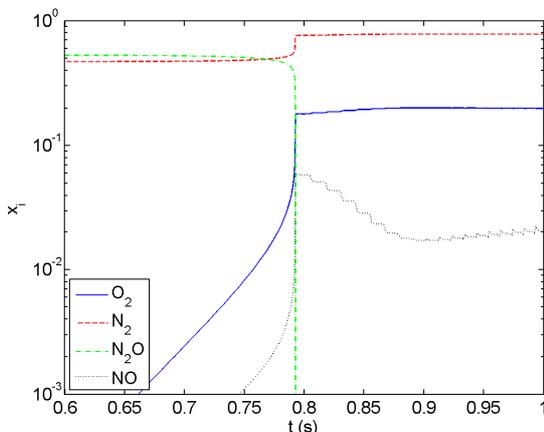

Figure 7. Barrel temperature as a function of time.

Figure 8. Species mole fractions as a function of time for the N_2/N_2O case.

The temperature of the N_2/N_2O mixture does not increase as rapidly as the N_2/O_2 mixture (Fig. 7) prior to the thermal decomposition of N_2O primarily because the simulated mass of gas compressed in the N_2/N_2O case is larger by about 27 %. (The constant volume specific heats of N_2O and air are about the same initially.)

The mole fractions of the major species are presented in Fig. 8 for the N_2/N_2O case. There is rapid and almost complete decomposition of the N_2O at about 0.8 seconds after the valve is first opened. However, around this time, about 6 % of the total molecules present will actually be NO. The simulations indicate that the mole fraction of NO falls to about 2 % over the subsequent 0.2 seconds.)

5. Conclusion

Simulation of the free piston compression process for the Ludwieg tube with thermal decomposition of N_2O has been achieved. The simulation indicates that fluctuations of an intolerable magnitude are likely to arise due to the decomposition of the N_2O. The present simulation is somewhat deficient in that the actual wave processes that will be generated by N_2O decomposition have not been considered. These waves will affect the piston dynamics. Nevertheless, it will be necessary to consider alternative strategies to successfully implement thermal decomposition of N_2O as a means to increase the enthalpy of the test gas and produce an air-like medium suitable for supersonic combustion experiments. One approach might be to introduce a fixed volume which is fed by the piston through a check valve (in a manner similar to the long-shot wind tunnel) as has been done elsewhere. Another approach might be to use piston braking.

6. Acknowledgments

7. References

[1] R.J. Stalker, Aero J. **110** (2005) pp. 21-39.

[2] R.L. Williams, J. Aircraft **1** (1964) pp. 236-241.

[3] R.R. Craig and P.J. Ortwerth, AIAA J. **5** (1967) pp. 2271-2274.

[4] N.A. Anfimov, V.V. Kislykh, and K.V. Krapivnoy, AIAA Paper 93-2016 (1993).

[5] Bogdanoff, G.J. Wilson, and M.A. Sussman, AIAA J. **35** (1997), pp. 1048-1056.

[6] Shumskii and M.I. Yaroslavtsev, Combustion, Explosion & Shock Waves **43** (2007) pp. 518-529.

[7] J.A. Miller and C.T. Bowman, Prog. Energy Combust. Sci. **15** (1989), pp. 287–338.

[8] T.V. Jones, D.L. Schultz and A.D. Hendley, Aero Res Council, Reports and Memoranda No. 3731 (1973).