

# The Thermally-Induced Decomposition of High Pressure Nitrous Oxide, Argon, and Helium Mixtures in a Closed Vessel

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Development of alternative gas generating methodologies for application in automotive airbag applications has led to an inflator [1] that uses standard pyrotechnic initiators to heat a high-pressure mixture of compressed gases that includes nitrous oxide as one constituent, thereby inducing thermal dissociation of a portion of the stored nitrous oxide charge. Accordingly, it is of interest to understand the extent of nitrous oxide dissociation as a function of important system operating parameters such as temperature, internal pressure, gas mass, and magnitude of energy input into the system. In addition, it is desirable to develop a predictive model that accurately simulates the extent of nitrous oxide dissociation in physically-similar closed systems, wherein the dissociation is initiated by imparting a well-characterized energy input into a compressed gas mixture. There were two main objectives of this work: First, to characterize system performance, experimental measurements of the extent of nitrous oxide dissociation in closed vessels for three component (N<sub>2</sub>O/Ar/He) gas mixtures were required as a function of temperature (-40°C to 90°C), initial pressure (1.72 to 13.79 MPa), nitrous oxide concentration (10% to 50%), and initial gas density (0.015 g/cc to 0.275 g/cc). The second objective was to develop an analytical model capable of accurately predicting the rate of pressure rise and the extent of dissociation of nitrous oxide in closed vessels.

The first step in understanding and modeling the extent of nitrous oxide dissociation in closed vessels was to characterize the energy introduced by the initiation source. Results from this work have been presented previously [2], where we disclosed experimentally-derived values for the amount of energy released by the discharge of zirconium potassium perchlorate (ZPP) and titanium hydride potassium perchlorate (THPP) initiator pyrotechnic formulations into pure helium environments. More recently [3], we have reported values of the extent of nitrous oxide dissociation as induced by 275 mg ZPP and 460 mg THPP initiators as a function of temperature and pressure, but only for mixtures containing 70% argon, 20% nitrous oxide, and 10% helium. The extent of dissociation “ $\epsilon$ ” was defined as the residual nitrous oxide in the test vessel after discharge of the

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initiator, heating of the compressed gas charge, dissociation of a fraction of the stored nitrous oxide, and subsequent equilibration of the reaction products and test fixture to the ambient temperature. One major finding of this study was that as the initial pressure within the test vessel increased (and initial density therefore increased) the extent of dissociation was generally found to decrease. In the absence of both additional experimental data and an analytical model, one conclusion drawn was that heat transfer to the walls of the test vessel, as well as the progressively higher gas densities, effectively quenched the dissociation reaction such that the extent of nitrous oxide dissociated was limited to relatively low values. However, it was pointed out that this may not be the case given larger energy inputs and increased initial nitrous oxide concentrations. Clearly more experimental data – primarily at higher nitrous oxide concentrations – and a predictive model incorporating appropriate kinetic and heat transfer terms would be beneficial to substantiate these conclusions. Thus, general of addition experimental data and the development of first generation predictive model were the specific objectives of the work reported here.

Tests were conducted in a specially-designed, 100 cc volume, closed vessel apparatus. The mechanical details of the design of the test fixture, illustrated in Figure [1] have been previously disclosed [2]. Gases were introduced individually into the fixture on a mass basis to ensure accurate mixture concentration and mass load. The extent of dissociation “ε” was determined through use of the gas fill information in conjunction with the measured mole fractions of nitrous oxide, oxygen, and nitrogen present in the reaction products as measured by FTIR and GC/MS instrumentation. The results illustrated in Figures 2 and 3 are indicative of those obtained in the experimental work. Note, as may be expected, the extent of dissociation is observed to increase the initial temperature of the mixture increase

A simple constant volume reactor model, primarily based on the work of Turns [4], was developed to describe our results. The assumptions in this model were:

- 1.) The reactor volume and the total mass the internal contents were considered constant.
- 2.) A real gas BWR (Benedict-Webb-Rubin) equation of state based on earlier work [5] was used to describe the P-v-T behavior of the initial gas mixtures.
- 3.) The primary mode of heat transfer, to the extent it occurred, was via radiation.
- 4.) Internal equilibrium states were assumed to be established instantly, so a well-defined thermodynamic temperature and pressure could be defined at all times
- 5.) The reacting gas mixture was well-stirred and homogeneous at each instant
- 6.) A single, forward chemical reaction step was used to describe nitrous oxide dissociation.
- 7.) The initiator was assumed to introduce energy into the gas mixture instantaneously throughout the initial gas mixture in a uniform manner.

The model reduced to the following set of ordinary first-order differential and auxiliary equations to be solved numerically [4]:

$$\frac{dT}{dt} = \frac{Q(V)^{-1} + R_u T \sum \omega_i - \sum (h_i \omega_i)}{\sum [(X_i)(c_{p,i} - R_u)]}$$

$$\frac{dX_i}{dt} = f_i(X_i, T)$$

$$d[X_i]/dt = \omega = g[(X_i), T]$$

$$dP/dt = R_u T \sum d[X_i]/dt + R_u \sum [X_i] dT/dt$$

$$-\sum h_i \omega_i = -k[N_2O] \Delta H_{rxn}(T)$$

where:

$R_u$  and  $V$  are the Universal Gas Constant and the test vessel volume, respectively

$P$  and  $T$  are the system internal pressure and temperature, respectively

$C_{p,i}$  is the constant pressure specific heat capacity of the  $i^{\text{th}}$  species

$h_i$  is the molar enthalpy of the  $i^{\text{th}}$  species

$(X_i)$  is defined as the molar concentration of the  $i^{\text{th}}$  species

$Q$  is the heat transfer rate to the test vessel walls

$k$  is the high pressure unimolecular rate constant

$\Delta H_{rxn}(T)$  is the heat of the decomposition reaction at the temperature ( $T$ )

Comparisons of the predicted extent of nitrous oxide dissociation and internal pressure with experimental data are presented in this work. Results obtained from the predicted code yield accurate results for a number of experimental conditions.

#### References

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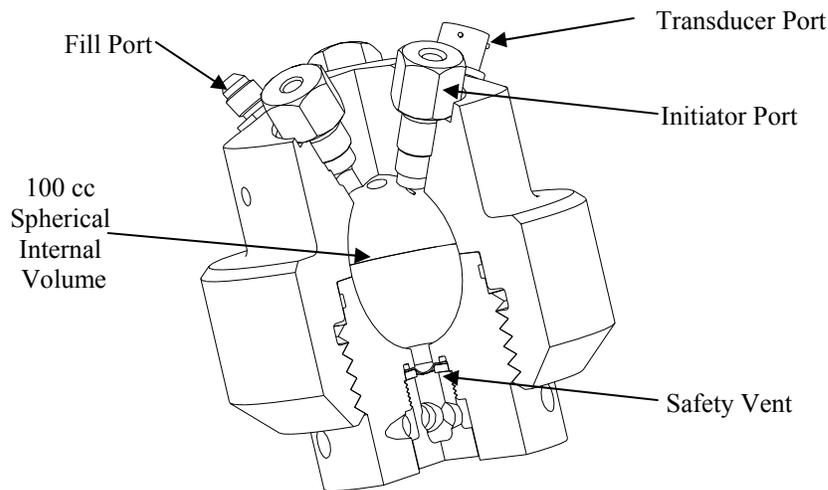


Figure 1. Important features of the test fixture design.

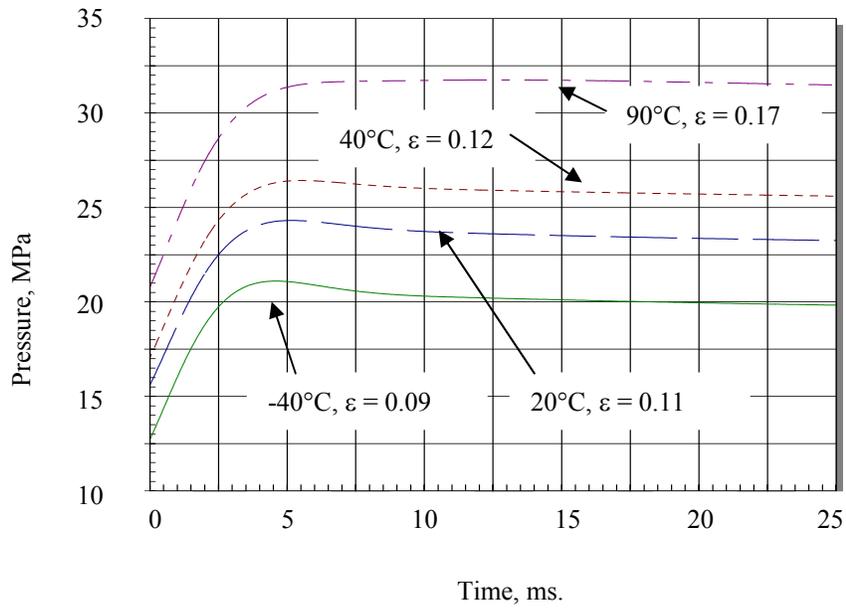


Figure 2. The effect of temperature on internal pressure and extent of nitrous oxide dissociation induced by a 275 mg ZPP initiator discharged into 20.5 g of 70/20/10 N<sub>2</sub>O/Ar/He.

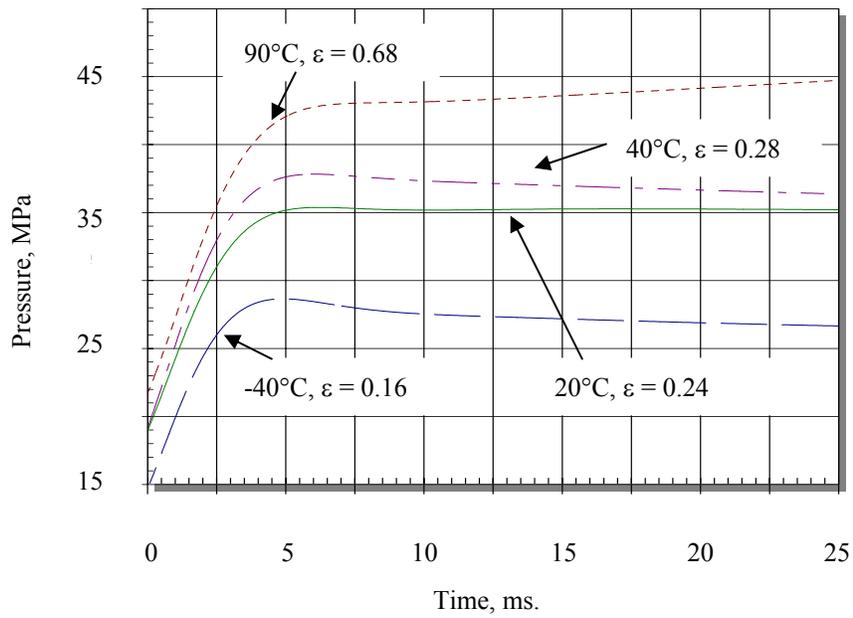


Figure 3. The effect of temperature on internal pressure and extent of nitrous oxide dissociation induced by a 460 mg THPP initiator discharged into 20.5 g of 70/20/10 N<sub>2</sub>O/Ar/He.