

# Failure analysis of a pressure vessel subjected to an internal blast load

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## ABSTRACT

The objective of the current work is to model a stainless steel (SA 316L) autoclave explosion and rupture that occurred during a research laboratory experiment designed to study the thermal decomposition of ammonium tetrathiomolybdate in the presence of dimethylsulfoxide (DMSO) in the autoclave. A finite element analysis is conducted to better understand the cause of failure of the autoclave and with the objective to investigate whether the incident was caused by static overpressure or an internal blast load. The empirical CONWEP blast loading model is used to model the internal blast load. The constitutive behavior of the autoclave material is modelled using the Johnson-Cook (JC) plasticity and material failure model, which both account for the effect of strain rate and temperature. By conducting uniaxial tensile tests and tests on notched ring specimens cut from the autoclave, the true stress-strain curve and the ductile failure locus of the autoclave material are established, respectively, which are used to obtain the constants of the JC plasticity and failure model, respectively. The result of the finite element analysis revealed that a blast load from an equivalent TNT charge of 0.042 kg, which resulted from the decomposition of DMSO at high temperature, predicted markedly well the structural response and subsequent failure of the autoclave observed in the post-incident investigation.

## 1. Introduction

Pressure vessels [1] and autoclaves are commonly designed to resist overpressure to a certain extent. Autoclaves used to conduct chemical experiments at high temperature and pressure are usually designed with a safety feature in the case of overpressure. Commonly, either a rupture disc is part of the vessel or the bottom part of the autoclave is designed to shear off such that excess pressure can be released, in addition to optional provision of pressure relief valve [2]. However, certain explosive chemical reactions can proceed with a speed such that the shock wave created from the explosion may rupture the autoclave before any of the pressure relief mechanisms can release the excess pressure.

Chemical explosions [3] involve rapid reaction of oxidizers and fuel components that comprise the explosive mixture. There is a sudden release of energy with the explosion, which produces a shock wave that propagates outward from the center of the explosion. Fig. 1 shows a typical form of a blast wave after a chemical explosion. The pressure pulse is often characterized by a sudden increase in pressure from ambient pressure,  $P_o$  to a peak incident overpressure  $P_{so}$ . The overpressure decays exponentially as shown in Fig. 1, and generally decreases to the ambient pressure in time  $t_o$ , referred to as the positive phase. This is followed by a negative pressure phase which is often neglected in blast loading calculations as little data exists for this regime. The area under the curve for the

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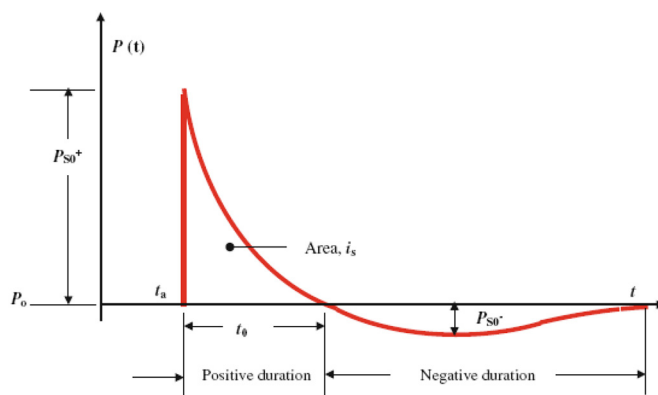


Fig. 1. Blast wave profile (pressure vs. time history) of an explosion [4].

positive phase is known as the specific impulse  $i_s$ . The peak overpressure, positive phase duration, and specific impulse are of particular interest in blast loading calculations.

In the current study, numerical modelling of an autoclave subjected to an internal blast load, resulting from an explosive chemical reaction, is undertaken. The purpose is to simulate the failure scenario of an incident that occurred in a chemical laboratory while conducting an experiment to decompose ammonium tetrathiomolybdate (ATM) and carbon nanotubes using dimethyl-sulfoxide (DMSO) as a solvent. Reactants in the ruptured autoclave, henceforth referred to as autoclave 'A', contained 33 mg ATM, 100 mg of carbon nanotubes and 65 cm<sup>3</sup> of DMSO as solvent. The reactants in the other autoclave, henceforth referred to as autoclave 'B', were the same, but with 65 cm<sup>3</sup> of water as solvent instead of the DMSO. Both experiments were conducted using Teflon®-lined reaction autoclaves (125 ml capacity each) made of SA 316L stainless steel, manufactured by Parr Instrument Company [2]. The autoclaves (model number 4750) are designed to operate below a temperature and pressure of 350 °C and 20 MPa, respectively. Both vessels were equipped with means to attach a pressure relief valve, but this was not used during the experiment. The autoclaves were placed in a bench top furnace where temperature was programmed to increase at a rate of 5 °C per minute from room temperature to a final steady state temperature of 300 °C. The experiment was expected to run for 72 h, but an explosion occurred at approximately two hours into the experiment. This resulted in the rupture of the autoclave 'A', causing significant damage to the furnace and the fume hood as shown in Fig. 2, luckily without any injuries to laboratory staff as they were out of the lab when the explosion occurred. DMSO is commonly used as a solvent in many chemical reactions [5–7], however it is also known to be thermally unstable due to its low auto-ignition temperature of 215 °C and undergoes an exothermic reaction when decomposed. This is especially true when heated above its decomposition temperature in the presence of an ammonia-generating compound, which can lead to a violent exothermic reaction and a subsequent explosion.

Numerical analysis of equipment subjected to blast loads requires a detailed understanding of the blast phenomena, the dynamic response of the material and subsequently the failure mode of the material involved. The Conventional Weapons Effect Program (CONWEP) blast loading model, was developed for military purposes, and is a collection of conventional weapons effects calculations from empirical relationships and curves found in TM5-855-1 [8]. The input parameters needed to model the blast load using the CONWEP model include a defined amount of Trinitrotoluene (TNT) charge at a given distance from the source of explosion, type of blast, detonation location, and surface identification for which pressure is applied. The CONWEP model also takes into consideration the reflected pressure, and the total blast pressure is calculated using



Fig. 2. (a) Damage caused by the ruptured autoclave 'A' (containing DMSO as a solvent) to autoclave 'B' (containing water as a solvent) and (b) damage caused to the furnace and the fume hood.

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