Explosive Characteristics of a Typical Li-ion battery Vent Gas with Inert Gas Addition

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1 Introduction

Li-ion batteries are one of the most advanced rechargeable batteries and differentiate themselves from other traditional batteries by containing high energy density, low self-discharge, and low maintenance [1, 2]. Due to the possibility of the release of combustible materials, these batteries create safety concerns. An inert gas extinguishing system has been tested for handling battery fires by reducing the oxygen concentration to approximately 12 vol% [3, 4]. However, it is not certain that reducing the oxygen concentration to about 12 % will remove the potential of an accidental explosion. To evaluate the effectiveness of Inergen, this study will determine the lower and upper explosive limits (LEL, UEL), the rate of explosion pressure rise, and the maximum explosion pressure for a typical Li-ion vent gas in the air, with the addition of an inert gas.

2 Materials and Methods

Figure 1 shows the 20-liter explosion sphere that was used in this experimental campaign. The experimental setup and procedure have been published previously [2]. It consists of an insulated steel sphere with a heating jacket that controls the temperature in the sphere. Two 601CAA Kistler pressure transducers measure the explosion pressure. A Keller PAA-33X pressure transducer was used to record pressure during filling. The pressure was logged throughout the filling process in order to get the filling pressure for each component. The explosion sphere had two separate injection ports, one dedicated to oxidizer and another for filling both inert and fuel. The port for both inert and fuel was flushed when switching from one gas to the other. The exploding/fusing wire method was used to ignite the mixture. The temperature and pressure set-point for all experiments were chosen to be 300 K and 100 kPa absolute, respectively.

Before each experiment, the explosion sphere was purged with compressed and oil-free air for ten minutes to remove any unwanted components from the previous experiment. The wire ignition system was implemented by setting the ignition coil before sealing the explosion sphere. Afterward, the explosion sphere was lowered to an absolute pressure of 10 kPa. Thereafter, the fuel and inert were filled to the desired partial pressure before filling it with air to 100 kPa. To ensure a homogeneous mixture, the gas mixture was actively mixed for five minutes before recording the temperature. To make sure that the mixture was quiescent, the ignition was delayed three minutes after mixing. For several of the experiments measuring the explosion pressure and the maximum rate of explosion pressure rise, parallel experiments were performed to see the variance in the results. As for the explosive limits, two parallel experiments with no ignition were conducted. Table 1 shows the gas compositions used in this study.

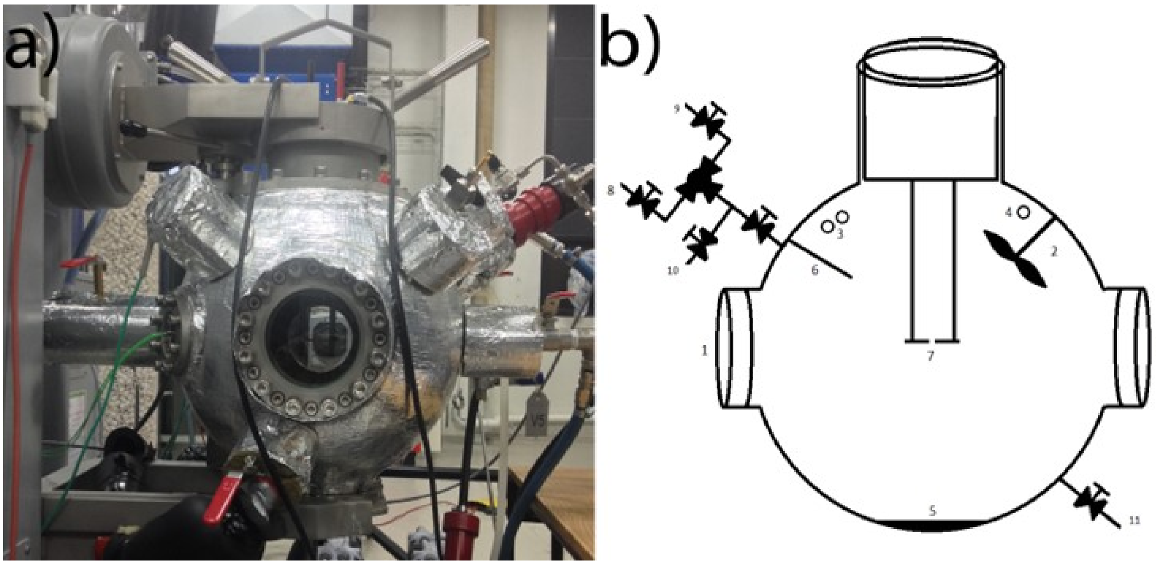

Figure 1: A photo (a) and an illustration (b) of the 20-liter explosion sphere [2]. 1: Windows; 2: Stirrer; 3: Two Kistler Transducers; 4: Keller Pressure Transducer; 5: Heating Plate; 6: Temperature Sensor; 7: Ignition Electrodes; 8: Fuel filling port; 9: Inert filling port; 10: Flushing port; 11: Oxidizer filling port.

Table 1: Compositions of gases utilized

Gas mixture name	Gas components
Generic Li-ion Gas	34.9% H_2, 10% CO, 30% CO_2, 20.1% CH_4, 5% C_2H_4
Inergen (IG-541)	52% N_2, 40% Ar, 8% CO_2

In a previous study by Henriksen et al. [5], a comparison of the combustion properties of several Li-ion vent gases was performed. The comparison showed that the Generic Li-ion gas had combustion properties within the range of most Li-ion vent gases. Therefore, the Generic Li-ion gas was chosen to represent a typical Li-ion vent gas in this study. The purity of all the gas mixture was within $\pm$ 0.1 % or lower.

Le Chatelier's principle was used to estimate the explosion limit, shown in Equation 1. For calculating the adiabatic flame temperature and the adiabatic closed-volume explosion pressure, the thermodynamic solver equilibrate in the Cantera [6] module for Python was used. The thermodynamic solver *equilibrate* finds the composition with minimum Gibbs free energy at constant internal energy and volume to calculate the constant-volume explosion pressure. The calculation requires a reaction mechanism model, which comprises the chemical kinetic, thermodynamic, and transport data of the included species and reactions as input. In this study, the Gri Mech 3.0 [7] was used.

$$X_{(LEL,UEL),mix} = \frac{1}{\sum_{i=1}^{n} \frac{X_i}{X_{(LEL,UEL),i}}} \quad (1)$$

Where $X_{(LEL,UEL),mix}$ is the volume fraction at the lower or upper explosive limit for the gas mixture, respectively, X_i is the volume fraction of component i, and $X_{(LEL,UEL),i}$ is volume fraction at the lower or upper explosive limit for species i.

The intended purpose of using an explosion and fire mitigation system, such as Inergen (IG-541), is to keep the oxygen concentration above the limit so humans do not faint and suffocate, while low enough to mitigate the explosion hazard. A possible method of achieving the target oxygen concentration is to inject a pre-calculated amount of inert gas that will displace a certain fraction of the air in the room. Therefore, the explosive limit is also given as a function of fuel concentration and the inert to air relation (α) given by Eq. 2. Where an α value of 0.5 is an equal concentration of air and inert in the total gas mixture.

$$\alpha = \frac{X_{inert}}{1 - X_{fuel}} \tag{2}$$

In this equation, α is the relation between inert and air, X_{inert} is the volume fraction of inert, X_{fuel} is the volume fraction of fuel.

The adiabatic flame temperature at the lower and upper explosive limits is used in the algorithm as a threshold to determine combustion at their corresponding limits. Le Chatelier's equation is used to estimate the explosive limits. Thereafter, the adiabatic flame temperature at each concentration is calculated using the equilibrate solver in Cantera at constant enthalpy and pressure, using the GRI 3.0 mechanism [7]. In this calculation, the lower and upper explosive limit and adiabatic flame temperature were estimated to be 6.5 % 995 K and 48 % and 1008 K, respectively.

3 Results and Discussion

Figure 2 illustrates the theoretical and numerical maximum explosion pressures and the maximum rates of explosion pressure rise as a function of fuel-air equivalence ratio (Φ) at different values of α.

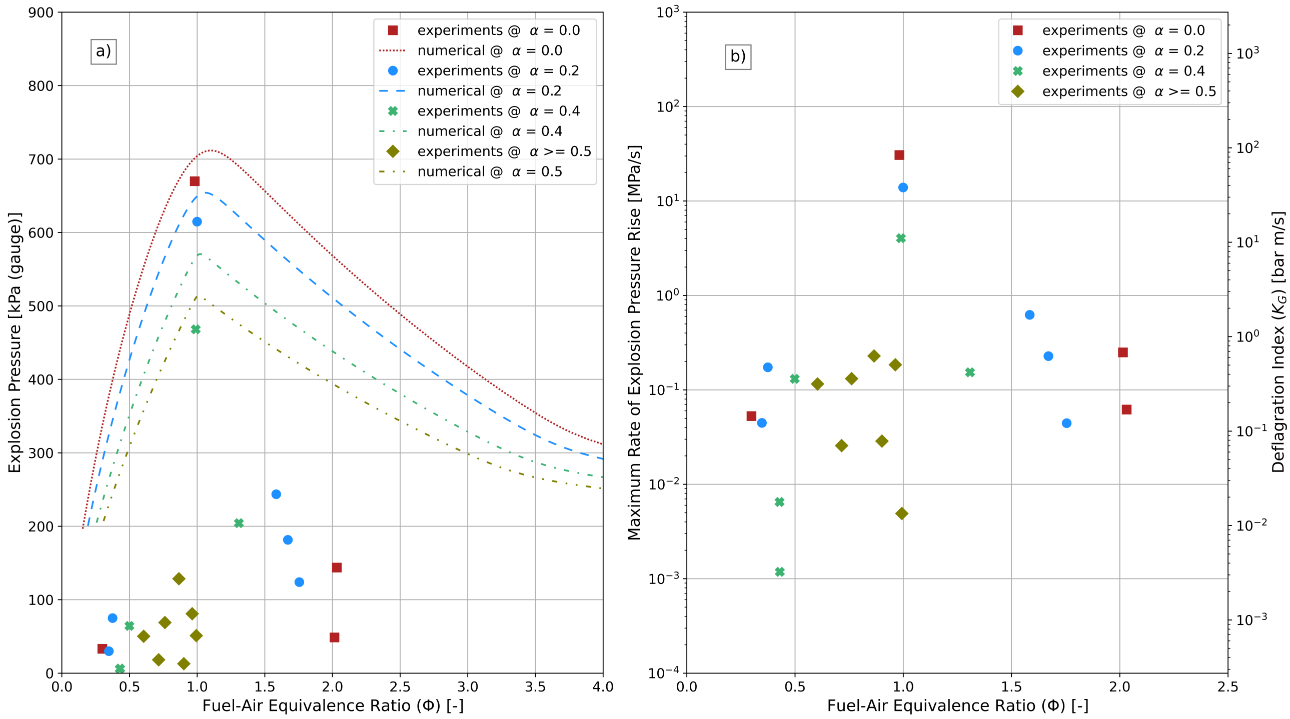

Figure 2: Theoretical and experimental maximum explosion pressures and maximum rates of pressure rise at 300 K and 100 kPa (absolute). a) Explosion pressure as a function of Φ; b) Rate of explosion pressure rise and Deflagration Index as a function of Φ

The explosion pressure decreases as the inert-to-air relation (α) increases, as expected. To effectively reduce the explosion pressure, the α should be higher than 0.4, and close to 0.5. At an α value of 0.4, the explosion pressure is reduced by approximately 200 kPa compared to a gas mixture without inert at a stoichiometric mixture.

The numerical and experimental results in Figure 2 a) agree well for the cases where Φ equals 1.0 and α is 0.2 or lower. Furthermore, the deviations at α of 0.4 and higher are believed to be caused by an increase in radiative heat loss and heat loss to the vessel walls. In contrast, the numerical explosion pressures are calculated for adiabatic conditions.

Figure 2 b) shows that the addition of Inergen has a more significant impact on the rate of explosion pressure rise. At an α of 0.4, the maximum rate of explosion pressure rise is reduced by an order of magnitude. When the α is increased to 0.5 and higher, the rate of explosion pressure rise is reduced to that near the explosive limit, when the mixture is without the addition of Inergen.

Figure 3 shows the numerical and experimental results of the explosive limit of the Generic Li-ion vent gas. The results in Figure 3 show that the numerical model, when using the explosive limits determined by Le Chatelier's (grey dashed line) agrees with the lower explosive limit for α values below 0.4. However, the model clearly over-predicts the explosive range, especially along the upper limit, which causes the extended explosion range at α and Inergen concentration above 0.6 and 55 %, respectively. It is well known that Le Chatelier's equation is less successful at predicting the upper explosive limit, which the present results also show.

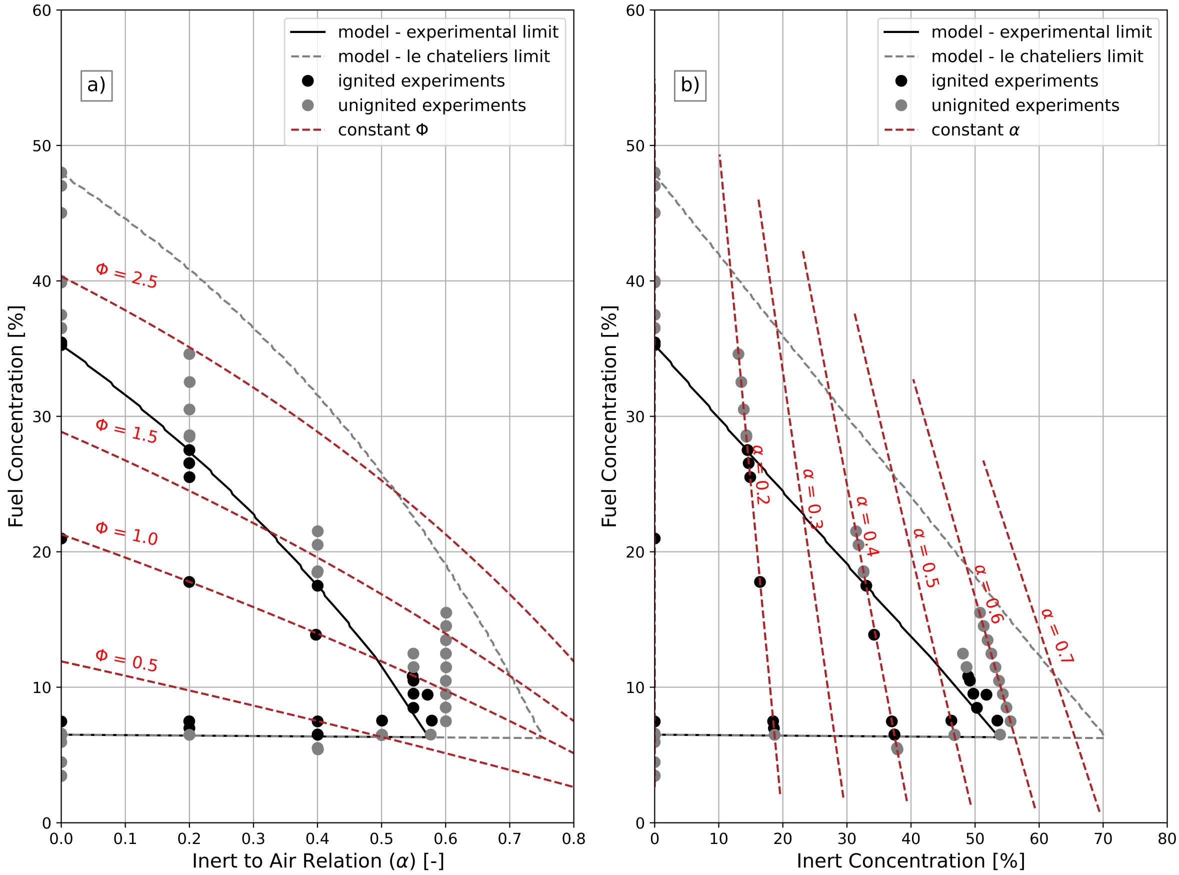

Figure 3: Preliminary numerical and numerical results of the explosive limits. a): Explosive limit as a function of α and fuel concentration; b):Explosive limit as a function of inert and fuel concentration

Updating the model with the explosive limits obtained from the experiments (black line) gives a much better agreement with the experimental results as inert is added to the mixture. However, as the mixture approaches the minimum inert concentration (MIC), the model starts to under-predict the explosive range. As the upper and lower explosive limit approaches each other, it may not be applicable to use a fixed adiabatic temperature as an ignition threshold.

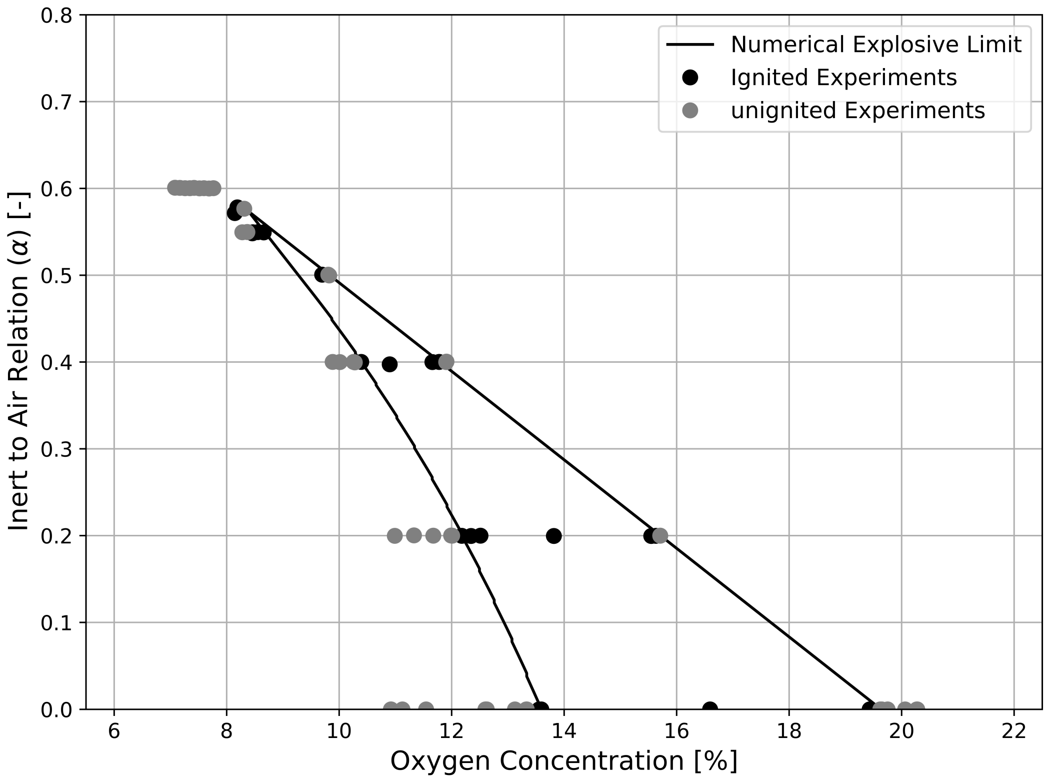

Figure 4: Numerical and experimental explosive limit as a function of oxygen concentration and α.

Figure 4 shows the numerical and experimental results of the explosive limit as a function of oxygen concentration and α. The oxygen concentration at the upper explosive limit without any addition of inert is approximately 13.5 %. However, as the α increases, explosions can occur at lower oxygen levels than 12 %. This indicates that reducing the oxygen concentration to only 12 % will not be effective in completely mitigating the explosion hazard. Furthermore, the experimental results show that the mixture is able to ignite at an oxygen concentration of almost 8 %. Both the numerical results and the experimental results show that inert will actually cause this battery gas to ignite at a lower oxygen concentration than without inert.

Finally, the results from this study show that using an inerting system with Inergen would not remove the explosion hazard. However, it will reduce the maximum explosion pressure and maximum rate of explosion pressure rise, thus potentially reducing the consequences of an incident.

4 Conclusion

In this experimental and numerical study, the explosion characteristics of a typical Li-ion vent gas was investigated using a 20-liter explosion sphere and the chemical kinetics, thermodynamic solver Cantera. The lower and upper explosive limits (LEL and UEL), the rate of explosion pressure rise, and the maximum explosion pressure for Li-ion vent gas in air and with the addition of an inert gas were determined at different concentrations. In addition, a simple numerical algorithm was developed to determine the explosive limit with and without Inergen, using the adiabatic flame temperature as a criterion for ignition determination.

As expected, the explosion pressure and rate of explosion pressure rise decreased as the concentration of inert increased. At an inert-to-air relation (α) of 0.4, the explosion pressure and rate of explosion pressure rise were reduced by 200 kPa and a factor of 10, respectively. However, the oxygen concentration at these conditions is below the suggested inerting limit of 12%

The experimental and numerical results of the estimated explosive limits as a function of fuel concentration and the α show that the Li-ion gas can ignite below an oxygen concentration of 12 %. Furthermore, the results also show that the explosive limits for the Li-ion gas could ignite at lower oxygen concentrations when Inergen is mixed with air. Finally, although Inergen will not remove the explosion hazard, it can potentially reduce the consequences of an explosion.

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