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Reactive Chemicals

Ethylene Oxide/ Contaminant mixtures: highly reactive

Ethylene oxide (EO): Hazardous chemical!

EO hazard diamond

EO reactions proceed mainly via ring opening and are highly exothermic. Under appropriate conditions, EO is known to undergo a variety of reactions, such as isomerization, polymerization, hydrolysis, combustion, and decomposition, which produce considerable energy. Moreover, pure EO with a flash point of – 18 ^{o}C can be ignited without air or oxygen.

Despite the hazards, EO is an important industrial chemical and has been involved in serious incidents resulting in major damages as well as fatalities. Contamination is a significant factor in EO incidents.

Motivation:

- There are numerous industrial processes where EO can be contaminated by impurities, especially acids and bases.
- Many incidents have occurred where EO reacted with contaminants, which led to significant losses.
- Only a few studies has been undertaken to provide useful information of EO thermal behavior in the presence of impurities, especially acids and bases. Only one published research study reports measurements of EO and NaOH solution. There has been no published research of EO contaminated with KOH, ammonia hydroxide, or acid.

Proposed Research:

Measurements of EO reactivity in the presence of four different contaminants (KOH, NaOH, NH_4OH, and EDTA)

Objectives:

The main objective of this project is to build simulation models for the scenarios of EO in contact with contaminants. These models can represent the measured data as well as predict the explosive hazard of EO at typical operation conditions in industry to help guide EO process safety design.

To achieve the above objective, several steps will be performed in this project:

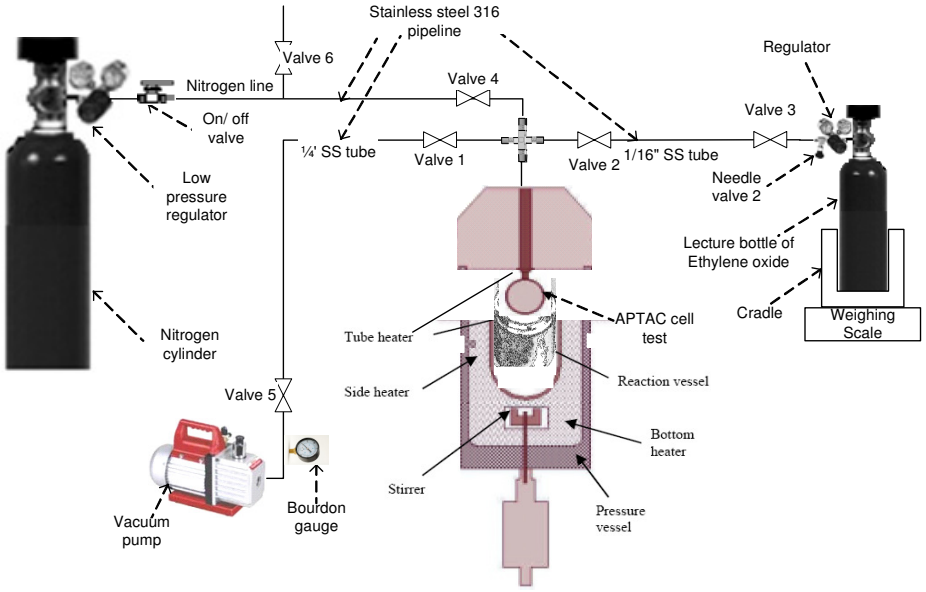
Step 1: Measure key exotherm parameters for EO in the presence of a wide range of contaminant/EO ratios using the Automatic Pressure Tracking Adiabatic Calorimeter (APTAC).

Step 2: Develop mechanism and kinetic models for the reactions of EO with different contaminants based on the EO experimental results and using computational methods.

Step 3: Based on the proposed mechanism and kinetic models, develop EO simulation models.

Experimental apparatus:

The special apparatus to transfer and measure the weight of the EO sample is shown in the following figure:



Initial results:

Based on the initial results, the following figure demonstrates some ideas about the effects of contamination on EO reactivity.