12th February 2025

Project Title

To generate the thermal hazard and process safety assessment data of industrial chemical reactions using reaction calorimeter (RC) and thermal screening unit (TSU).

Objectives

1. To conduct the reaction calorimeter experiment of industrial chemical reactions to generate the heat of reaction, heat rate, adiabatic temperature rise (∆Tad), maximum temperature of synthesis reaction (MTSR), and pressure rise data due to cooling failure.
2. To conduct the thermal screening experiment of industrial chemical reactions to generate important thermal hazard data such as reaction onset temperature, rate of temperature rise (dT/dt), rate of pressure rise (dP/dt), maximum possible pressure (Pmax), time from exotherm to explosion, etc.
3. To assess the safe storage and transportation conditions of chemicals.
4. To determine the range of safe operating parameters for a chemical process.

Executive summary

Process safety assessment of a chemical process at the plant scale is very important nowadays for safe operations. In the absence of this information, the chances of accidents are very high. We can see so many accidents in the news due to the explosion of reactors in terms of the release of temperature and pressure energy.

At CSIR-NCL we have a full-fledged RC and TSU facility, which can take industrial reaction samples to generate the required safety data. The heat of reaction, heat rate, ∆Tad, MTSR, pressure rise due to cooling failure, reaction onset temperature, (dT/dt)max, (dP/dt)max, Pmax, time from exotherm to the explosion data can be generated as consultancy industrial projects. The generated RC and TSU data will help the chemical industry with a safe scale-up of exothermic processes. It will also help to choose the safe range of operating parameters such as reaction temperature and pressure. It will also help for the safe storage condition assessment of various chemicals with thermal hazard nature.

For the RC study, the operating temperature range would be from 0 ºC to 160 ºC, and the pressure range would be from ambient to 40 Bar. For the TSU study, the operating temperature range would be from ambient to 300 ºC, and the pressure range would be from vacuum to 80 Bar. Almost all kind of industrial chemical reactions such as hydrogenation, nitration, grignard, hydrolysis, neutralization, etc can be conducted using RC and TSU facility at CSIR-NCL. However for reactions with corrosive nature, corrosion data would be required to check the feasibility. Similarly for high potent chemical reactions, exposure limit data would be needed to check the feasibility.

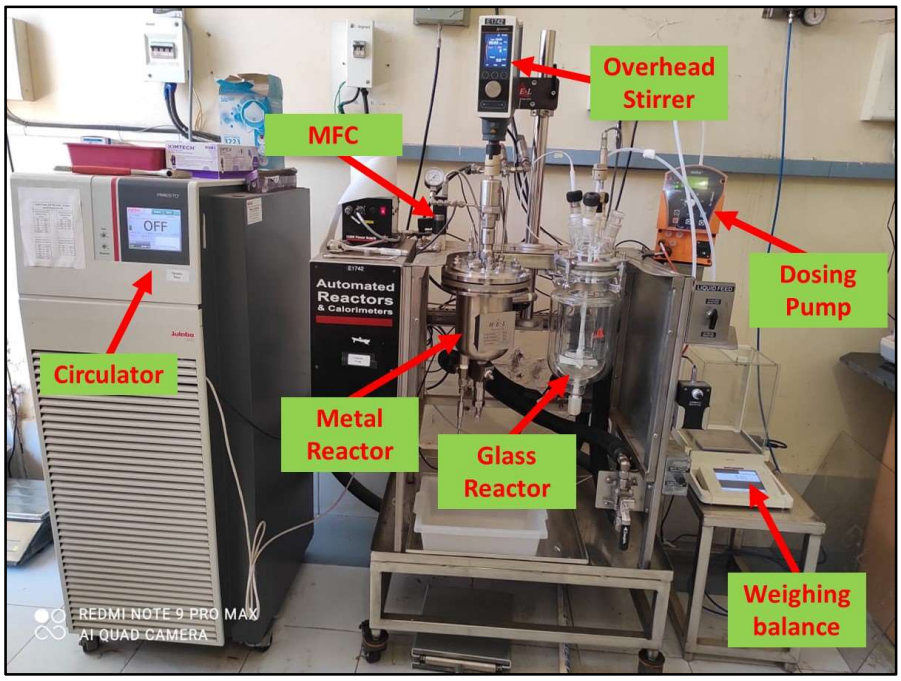

Figure 1: Reaction calorimeter experimental setup at CSIR-NCL Pune

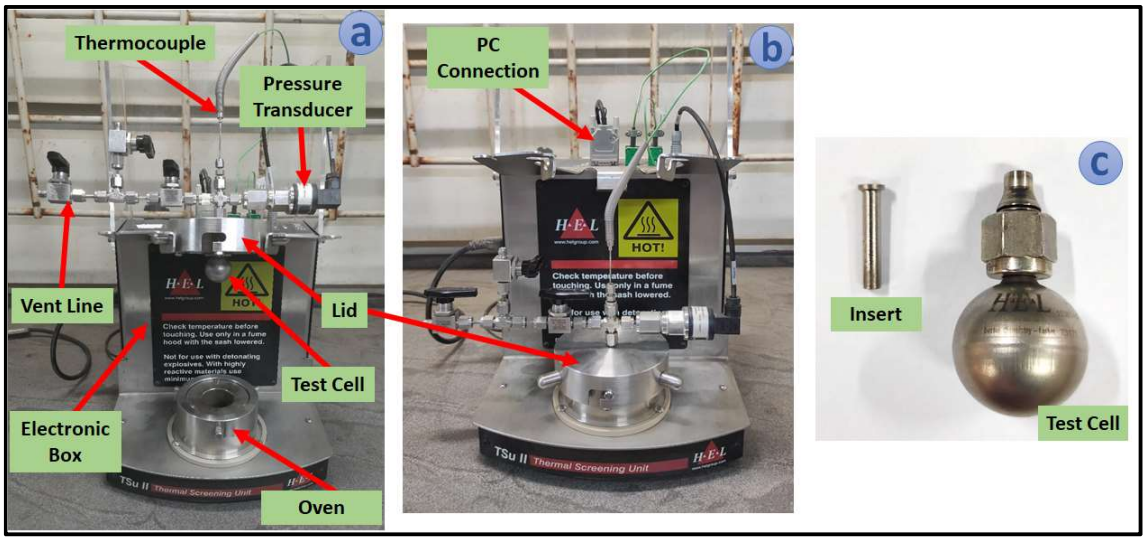

Figure 2: Picture of TSU setup at CSIR-NCL Pune; (a) TSU with test cell attached; (b) TSU with closed lid; (c) Hastelloy test cell and insert

Project Cost: As CSIR-NCL Pune already has this facility, hence only nominal testing charges to operate this facility would be required to avail this facility.

Project Duration (In months): 1 or 2 weeks after getting the required chemicals for the RC and TSU testing.

Deliverables

1. The heat of reaction, heat rate, ΔTad, MTSR, pressure rise due to cooling failure, reaction onset temperature, (dT/dt)max, (dP/dt)max, Pmax, time from exotherm to the explosion data generated from RC and TSU.
2. To train the chemical industry on how to use RC and TSU data for their processes for safe operation and for the selection of suitable MOC of their equipment such as reactor MOC.
3. To help the chemical industry to choose the safe range of operating parameters such as reaction temperature and pressure.
4. To help the chemical industry with the safe storage condition assessment of various chemicals with a thermal hazard nature.
5. To help the chemical industry to choose the safe reagent feeding rate and suitable chilling capacity for the exothermic industrial chemical processes.

Team detail

Sr. No.	Name	Role	Designation	Contact details
1	Mr. Rajendra Kumar	PI	Sr. Scientist CSIR-NCL Pune	Phone: 020-25902735 Mob: 7875111463 Email: k.rajendra@ncl.res.in
2	Dr. Nilesh Mali	Co-PI	Pr. Scientist CSIR-NCL Pune	Phone: 020-25902176 Mob: 9422770593 Email: na.mali@ncl.res.in
3	Dr. Sanjay Kamble	Co-PI	Sr. Pr. Scientist CSIR-NCL Pune	Phone: 020-25902732 Mob: 9423055351 Email: sp.kamble@ncl.res.in
4	Dr. Santosh Ghuge	Co-PI	Sr. Pr. Scientist CSIR-NCL Pune	Phone: 020-25903018 Mob: 8826982445 Email: sp.ghuge@ncl.res.in