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GLOBAL TECHNICAL INFORMATION MANAGEMENT IN THERMAL HAZARD EVALUATION

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Abstract

One of the critical aspects of an effective reactive chemicals program in the chemical processing industries is the management of our technical and project information. With the continuing evolution of electronic tools for the generation, storage, and retrieval of this technical information, we have new opportunities to improve management of process safety information.

New approaches in the documentation of reactive chemicals information are described. The documentation method is based upon a 'living' project file organized along process unit operations. The project file captures the project safety information in an 'information mapped' format. The format provides a simple means to document issue definition, relevant data and information, application of information to resolve the issue, and lines of defense and prevention.

Keywords: information management, project documentation, thermal hazard evaluation, unit operations

Introduction

Thermal hazard evaluation in the chemical industry has focused heavily in the past on experimental methods and analytical data generation in support of safe chemical processing. The management of the data and the information obtained from such data has received less attention. However, in the current business climate of decreasing expert resources coupled with a strong drive to high productivity levels, how we develop and manage our thermal and flammability information, or reactive chemicals (RC) information, is of great importance.

Our current efforts in this field are designed to improve the thermal hazard evaluation process via a three-part, but integrated approach. The three parts are

1. Documentation and Retrieval of reactive chemicals issues and solutions: the Information Management document template
2. Improved representation of thermal hazard results: graphical presentation of chemical process and reactive chemicals data
3. Improved communication of information: sharing information via an 'Intranet' website

This publication reports on the first part of our information management efforts, the development and implementation of a document template for creating a reactive chemicals process technology package.

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The information management document template

Purpose and scope of the template

The first part of our information management approach involves the capture of decisions and related data in an electronic document. The decision making in Reactive Chemicals data generation and interpretation can usually be reduced to three levels of complexity.

Level 1 – Yes/No decisions are made regarding basic thermal stability.

Analytical work involves analytical screening experiments for exothermic and pressure generating reactions.

Level 2 – An unequivocal decision is not possible. Maybe more analytical work is needed, but lines of defense may mitigate hazard.

Resolution of issue involves a balance between implementing additional lines of defense and/or obtaining additional quantitative reactivity data.

Level 3 – It is obvious that more analytical data are required to understand hazards.

Information is needed on how much heat and pressure are produced by the reaction, how fast are they produced, and how to control them. Additional data must be generated and scaled to process conditions.

These decisions and the logical thought processes leading to the decisions are rarely documented during process scale-up. However, the questions are often asked several times during the development of a process. In addition, relating the analytical results to the chemical process requires a balance between the amount of effort we place in understanding the chemistry, kinetics and thermodynamics of reactions, and the extent and cost of implementing lines of defense and prevention in the process. For a process which begins in research at a laboratory scale, yet eventually progresses to full scale manufacturing there is a critical need to capture and retrieve resolution of RC evaluations throughout the life of the process. Much higher levels of productivity may be achieved by documenting thermal hazard issues and their resolution at each stage of development and build upon the previous knowledge acquired. This concept is represented pictorially in Fig. 1.

We have developed a standard document template to help us manage the reactive chemicals process information. When the template is filled with process and reactive chemicals information it is then referred to as a reactive chemicals technology package, or RC tech package. The concept for such a template and technology package arose out of the needs of both the analytical support and the process owners. It became apparent that in our partner interactions, for all stages of process development the analytical data were retained but issues, scenarios, and interpretations were often not documented. This resulted in a loss of productivity when that information needed to be regenerated at some later date during scale-up of the process.

Format for the template

Thus the primary purpose for the template was to facilitate the development of a reactive chemicals technology package. The aim was to improve productivity in Reactive Chemicals by documenting the evaluation thought processes, reducing data to information, and making that information available to RC community elec-

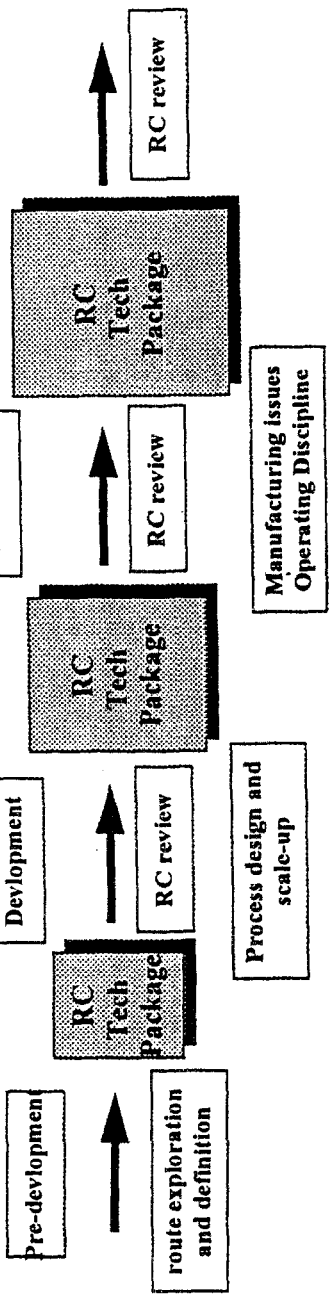

Fig. 1 The development of a reactive chemicals (RC) process technology package for the life of the process, from research to manufacturing stages

tronically in a common, easy to utilize format. The following attributes for the template were used to guide the development and implementation.

- simple, free format in outline form
- living, electronic document
- flexible, for large & small projects
- simple project management tool
- information-mapped format for quick assimilation and/or dissemination issues, plans, resolution, lines of defense
- contains prompts to serve as a 'checklist' of potential issues
- general resource for process safety information
- set up for inclusion of other pertinent information

The above attributes lead to the development of the following template. The information is organized under major headings which correspond with typical structuring of manufacturing information. To facilitate the navigation of the information, the sections are given as tables with headings to identify the nature of the contents of each block. The template gives guidance statements in each block to prompt the user to provide necessary information. Some sections are variable in length and are composed of repeating units which contain information of similar purpose. The largest repeating units are those of the unit operation and raw materials. Each of these sections are repeated for as many unit operations and raw materials as the process may contain. In addition to those large sections, there are subsections of each which are key to overall value of the finished document. These are the set of four blocks which are used to described 1.) a reactive chemicals issue of concern, 2.) the plan to obtain data or information relevant to the issue, 3.) the resolution of the concern via interpretation of relevant data in the context of the processing conditions, and 4.) the selected lines of defense to mitigate the initial reactive chemicals concern. These blocks allow the user to easily identify concerns and resolve them, document this issue and resolution, and provide a means to retrieve such information conveniently at a later date. The template is given below.

Reactive chemicals evaluation/documentation tool

Process name – example

Objectives	• Give the objectives of the project
Project team members	• List the key members of the project team, primary contact, phone, e-mail, address...
Timelines	• Give the timelines of the project (when must we be finished?)
Scale	• Give the volume of the largest vessel and the volume from which this process is being scaled-up
Chemistry	• Describe intended chemistry and include structures
Block flow diagram	• Attach on next page if large. Label stream with RC report numbers where applicable

Major reactive chemicals issues	• List the known major reactive chemicals issues and any previous incidents
Key lines of defense	• List the current or proposed lines of defense. For projects going to Third Party Contract Manufacturing, list these as 'Some Lines of Defense to Consider'.

Unit operation (#1)

Chemical reaction/distillation/crystallization/filtration/centrifugation/drying/etc...

Chemistry
• Show chemical reaction with structures (if applicable for this unit op)

Recipe
• List amounts and order of addition of materials (concentrations or unit ratios), process conditions (temperature, pressure, reaction times). List type of process (batch, con-add, etc.)

Steps	Example description	Temp./°C
1	Load reactor with 200 lb. A	25
2	Cool reactor to -10°	−10
3	Con-add 50 lb. B to maintain temperature at -10°	−10

Equipment
• Show vessel design along with associated piping and process equipment, especially safety equipment
• List materials of construction
• Safety relief
• Agitation
• Heat removal capability

Concern
• What is the reactive chemicals concern with the proposed operation. Define a credible reactive chemicals scenario
• For example, will loss of control of the desired synthesis reaction trigger an undesired decomposition reaction?

Plan
• (This plan is developed as a joint effort between the reactive chemicals and process personnel.) Describe plan(s) to obtain the necessary information to resolve the concern. Include type of data or information, quality of data, and final form of data needed.

Resolution
• List data pertinent to concern along with data source
• Describe data reduction and consequences to process operation
• After obtaining the necessary data, apply reactive chemicals data and information to concern
• Describe the conditions under which the reactive chemicals scenario can occur and what is expected to happen based upon the process conditions, the reactive chemicals data, and interpretation of those data.
• Define safe operating window: temperatures, pressures, compositions, reaction times, etc.
• Include engineering calculations performed by partner.

Lines of defense
• What lines of defense are in place to prevent or control the scenario?

Raw material storage and handling – An example

Raw material	Packaging	Appearance	ID method
Material #1	bulk – seatainer	pale yellow solid	IR/GC
Material #2	55 gallon drums	colorless liquid	
Material #3	22.5"×33.75" Fiber Pack	white powder	

Material #1

Thermal stability	• Describe thermal stability in nitrogen and air at ambient (storage) conditions. For example: Is the material susceptible to air oxidation? What is length of storage time? Is there temperature control?
Flammability	• Flash point, AIT, flammable limits (if known)
Reactivity	• Reactivity with other chemicals in process
Equipment and materials of construction	• Show vessel design along with associated piping and process equipment, especially safety equipment • List materials of construction • Safety Relief • Agitation • Heat removal capability
Safe handling guidelines	• Give pertinent information from manufacturer, MSD's Bretherick 'Handbook of Reactive Chemicals Hazards', Sax 'Dangerous Properties of Industrial Materials', and other sources of safety information
Spill mitigation	• List procedure for handling spills • Absorbents to use or avoid, e.g. never use clay absorbents with monomers, never use organic absorbents with H_2O_2, etc.
Concern	• What is the reactive chemicals concern with handling/storage of this material. Define a credible reactive chemicals scenario. See two examples below: • Insulation fires from solvent leaks and spills on electric-traced or operating lines at process temperatures • Fires in distillation columns
Resolution	• After obtaining the necessary data, apply reactive chemicals data and information to concern. For example: • Ran open-cut ARC's in air and modeled results for solvent loaded on mineral wool and cellular glass insulations. TNR's predicted to be...
Lines of defense	• What lines of defense are in place to prevent or control the scenario? A few examples for above concerns include: • Plan to boil up water into column packing prior to cleanout • Use Cellular glass insulation: materials wet surface without penetration and it is rated as a vapor barrier

General operations – an example

Instrumentation and computer control	• Describe the important aspects of your instrumentation and control which relate to reactive chemicals issues. For example: • Computer control of Process • Critical instruments • Redundant instruments on different circuit boards? • Abort programming? • Alarms (high limit, failure). Programming to avoid set point changes outside acceptable range?
Insulation	• Type(s), susceptibility to fires when soaked with process materials?
Waste streams	• Discuss the issues relating to storage and disposal of wastes. Include spill remediation, safety at destination, storage conditions (temperature, time, vessel), inadvertent mixing with other waste stream.
Vent streams	• Discuss issues related to vent streams, for example: • Flammability: vapors, solids oxidative runaway • Cross-reactions • Condensation • Corrosion • Interface to TOX/THROX
Carbon beds	• Include intended use of carbon beds, if applicable
Safety relief design	• Describe basis of safety relief design, document design and include references to design reports and conclusions
Training	• Describe scope and frequency of training program
Compliance	• Document resolution of previous reactive chemicals issues and considerations which arose through reactive chemicals reviews and audits
Future actions and plans	• Describe reactive chemicals issues which will be addressed in the future, how they will be addressed, when, and by whom. Develop 'to do' list for pre-start-up, after start-up, or upon scale-up:

Reactive chemicals data for process

An example of tabulated data with references

Report reference	Sample description	Test	Atm.	Endo/ exo	Start/ °C	Peak/ °C	End/ °C	Heat/ mJ mg^{-1}
RCM 95-0000	Compound xyz in toluene	DSC	N_2	nothing	–	–	–	–
			air	exo	253	292	320	–19
RCM 96-0000	Tertiary alcohol (solid)	DSC	N_2	endo	171	190	216	+29
			air	endo	173	189	214	+36

Application of the template

One of the groups which benefits the most from the information captured in the template is the process owners, what we often refer to as partners and clients. Depending upon the stage of development of the process, the partners may be R&D chemists, engineers, project managers for Pilot, Market Development, or Manufacturing Plants, or Third-Party Contract Administrators. In the development of a reactive chemicals process technology package, the thermal analysts play a very important set of roles as stakeholders and facilitators. They must develop issues with partner and discuss lines of defense, plan data strategy within the partner's timing and cost requirements, resolve issues based on data and scenarios, enter the resolution of issues in template on owner's fileserver, and to help finalize lines of defense.

Conclusions

This template has been applied to several different projects within this company, from large and complex processes entering production to simple small scale projects from research. In all cases both the process owners and the thermal analysts found the RC technology package very useful. In general the following benefits were found during the trial stage of the template. The template

- provides information electronically in a networked environment to improve accessibility, e.g. process development and operating discipline creation
- facilitates the globalization of process safety information and thermal hazard evaluation through sharing of information
- serves as a crisis response tool
- helps employees spend less time going over previously covered ground
- identifies critically evaluated data for each process step
- makes the reactive chemicals process more complete with fewer oversights
- may be used as a training tool for both analyst and partner
- can be used to document our accomplishments on projects

Some of the disadvantages of the template are that it can require some additional effort to enter the issues, plans, resolutions, and lines of defense into an electronic document. However, this effort is preferable to not documenting the information at all. There is also a significant cost issue in applying the template to an existing process where information is already documented in other formats. For large, complex processes, the conversion from the old format to the template may require significant amounts of professional time.

We anticipate that this template will find widespread use in our company in the next few years. It will also certainly continue to evolve as it is applied in more and varying processes and chemistries. Although the template has found success within our company, it has only been applied to relatively large scale processes during scale-up in the agricultural business arena and some contract manufacturing projects dealing with relatively simple organic reactions. This template may not be complete or adequate for other chemical processes or non-typical chemicals. The authors in no way imply that this template is complete or universal a universal tool in all reactive chemicals problems. It is not a substitute for quantitative risk assessment or detailed hazardous operation studies.