

# PreVent

*(Process Reaction Evaluation & Vent Assessment)*

*A structured procedure to reduce the need for an extensive reaction hazard assessment of a process. This technique permits a faster and more cost-effective mechanism for ensuring an effective basis of reaction safety using valid and proven engineering solutions - particularly if pressure relief is to be employed.*



RCI (Picture Courtesy of Mettler Toledo)

## THE CHALLENGE

"I have a process that I want to operate using an existing reactor, that is equipped with an emergency vent as the basis of safety. I do not want to modify the plant to cope with the process and I need to demonstrate that my existing vent is adequately sized or an alternative basis of safety is appropriate, to handle a credible runaway scenario and I need to do it quickly and cost effectively."

A HSE survey was undertaken in 1997 to evaluate emergency relief systems that were present on chemical reaction vessels operated by industrial companies. The findings indicated that:

- Design Institute for Emergency Relief Systems (DIERS) methodology, accepted best practice, was used by only a small fraction of the companies surveyed.
- Fewer than 50% of companies had performed a reaction hazard assessment and the worst credible scenario for relief design was often unknown.
- Less than 50% of vessels were used for a single product. The majority were multi-product reactors

Legislation dictates the need to establish reaction hazard management. Within Europe, recently introduced legislation has, for the first time, made specific reference to assessing and controlling exothermic reaction hazards and thermal instability hazards. In the UK, this legislation is provided by the Dangerous Substances and Explosive Atmospheres Regulations (DSEAR) 2002 whilst within the remainder of Europe the Chemical Agents Directive (CAD) applies.

The survey supports the need for a strategic assessment methodology for all reactors and processes. Difficulties arise in putting in place a robust and rigorous methodology that can reliably identify worst case scenarios and confirm the acceptability of existing relief systems for a wide variety of reactors and processes. With just 5 reactors and 15 processes, not an uncommon situation, a potentially bewildering matrix of up to 75 combinations can require assessment.

## PREVENT - THE CHILWORTH SOLUTION

DIERS methodology is the industry-accepted approach to emergency pressure relief for runaway reactions, chemical decompositions and other systems likely to discharge a multi-phase stream under relief conditions, and relies on the provision of experimentally derived kinetic and thermodynamic data. Chilworth Technology has built upon the DIERS methodology and developed a protocol to help operating companies assess whether their existing vent configurations are suitable as a basis of safety and, if not, what cost-effective options are available for obtaining a suitable solution.

# Process Reaction Evaluation & Vent Assessment (PreVent)

## ASSESSING THE HAZARDS

To assess the hazards of a chemical process, and to define a basis of safety for large scale manufacturing plant, three essential phases need to be considered.

### 1. Normal Process Characterisation

- Determination of the heat and gas evolution of the normal process.
- Determination of the thermal stability limits of raw materials, intermediates and products used in the process.

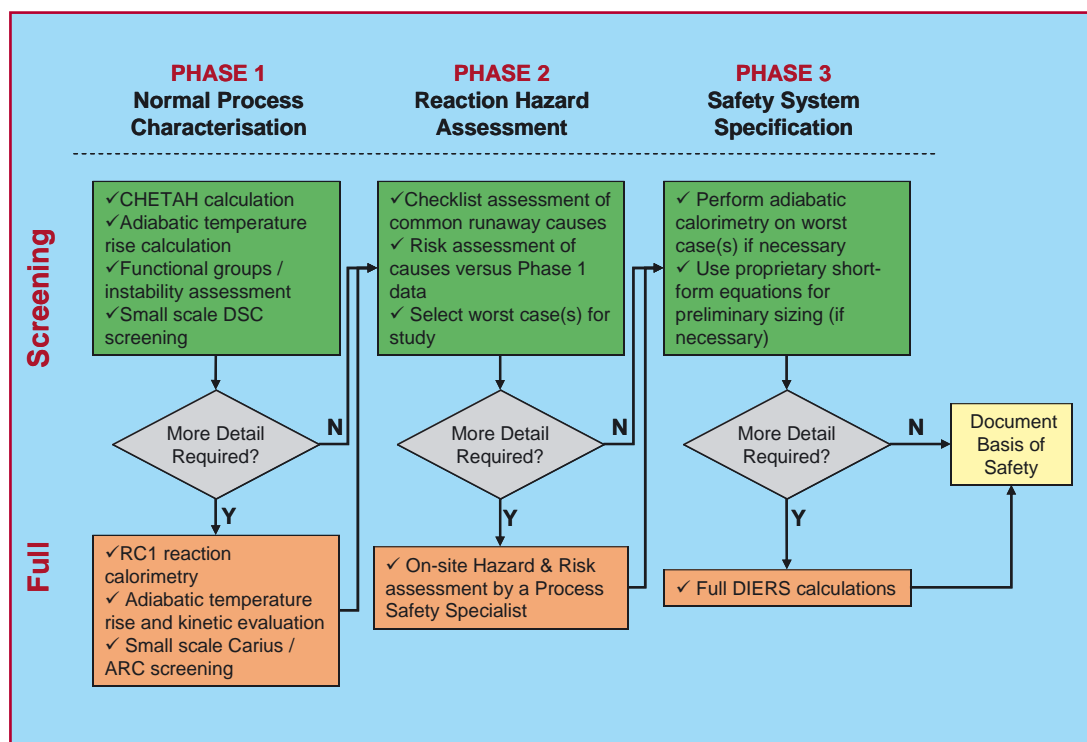
### 2. Reaction Hazard & Risk Assessment

- Hazard Identification : Examination of the proposed processing plant (along with the normal process information) to identify any potential (foreseeable) process deviations.
- Risk Assessment : Evaluation, through experimental simulation or calculation, of the potential risk posed by process deviations.

### 3. Safety System Specification

- Evaluation through adiabatic calorimetry, the consequences of the most hazardous process deviation(s).
- Specification of process control and emergency safety measures required to maintain the plant in a safe condition (through all foreseeable process deviations).

Chilworth Technology has developed a two-level methodology to conduct these stages of assessment. The two-level approach provides a highly cost-effective screening technique which can be applied to processes of "lower" risk, whilst the more detailed assessment is reserved for "higher" risk processes. The screening approach shown in the chart below, together with the applied margins, can yield reliable results that do not need confirmation from a detailed assessment. However, it is not always easy to identify "lower" risk processes in advance of an experimental assessment, so if the screening technique (PreVent screening stages 1, 2 and 3) indicates a high potential hazard, the analysis can easily switch from the "screening" to the "full" methodology.



## PREVENT PHASES AT EACH LEVEL

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### Phase 1: Normal Process Characterisation

The aim of this phase of the PreVent study is to characterise the thermodynamics of the chemical reaction and to evaluate the propensity of the process materials (raw materials, products and intermediates) to exhibit thermal instability under process conditions. This will encompass:

#### Screening Level

- Evaluation of molecular structures for thermal instability (self-reaction or decomposition).
- CHETAH calculations to evaluate the heat of reaction for the balanced chemical reaction (and any known side reactions).
- Evaluation of potential for permanent (non-condensable) gas formation.
- Combination of the predicted heat of reaction with estimated heat capacity information to allow estimation of the potential adiabatic temperature rise of the desired reaction including any known and specified side reactions.
- Estimation of the peak pressure at this maximum anticipated temperature, using component physical properties.
- Conduct and interpretation of small scale DSC testing.

#### Decision

Does the data obtained suggest more detailed analysis is required (go to "Full" Level) or does the data indicate a sufficiently benign system to proceed without experimentation (i.e. proceed to Phase 2)?

#### Full Level

- RC1 Reaction calorimetry on the normal process with coincident evolved gas measurement to fully characterise the heat of reaction, kinetics, power output, mixture heat capacity and gas evolution rate and quantity.
- Evaluation of the potential adiabatic temperature rise.
- Evaluation of molecular structures for thermal instability (self-reaction or decomposition).
- Conduct small scale thermal screening studies to evaluate decomposition potential (onset temperature conditions, magnitude, rate and coincident pressure effects).



### Phase 2: Reaction Hazard Assessment

This phase of the PreVent study will identify potential process deviations associated with the reaction, and then evaluate which of these can present a hazard. This will encompass:

#### Screening Level

- Generic hazard identification exercise using a checklist of common process deviations appropriate to the operation.
- Calculations to evaluate the overall consequence (magnitude) of process deviations (where possible) using data obtained at Phase 1.
- Selection of the appropriate scenario(s) for safety system design and identify the worst credible scenario(s) for emergency relief vent design.
- Comparison against the requirements of other processes operated in the same equipment.
- Chemical compatibility assessment across all processes - via prediction methods.

#### Decision

Does the data indicate a sufficiently robust and fault tolerant reaction can proceed without a more detailed hazard assessment? If not, perform a detailed on-site hazard assessment.

#### Full Level

- Build on the generic hazard identification exercise with an on-site hazard assessment performed by an experienced Chilworth Technology Process Safety Specialist. This will be a detailed and plant specific assessment.

## WHAT IS PREVENT AIMED AT?

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The methodology is intended to be applicable to almost any reactor / reaction combination. This will include:

- New processes in new reactors,
- New processes in existing reactors or
- Existing processes in new and existing reactors

Although it is predominantly aimed at multi-product plant, it can also be successfully applied to any situation where the scale-up of a chemical reaction occurs (either to pilot or full production scale).

The methodology is particularly applicable for the rapid screening of new processes entering existing plant where the vessel volume, design pressure, the relief device size and set pressure, and the proposed batch size are known or fixed.

## Phase 3: Safety System Specification

The final phase of PreVent characterises the consequences of worst case scenarios and provides data for the sizing of emergency relief systems or specification of other safety protection systems. This will encompass:

### Screening Level

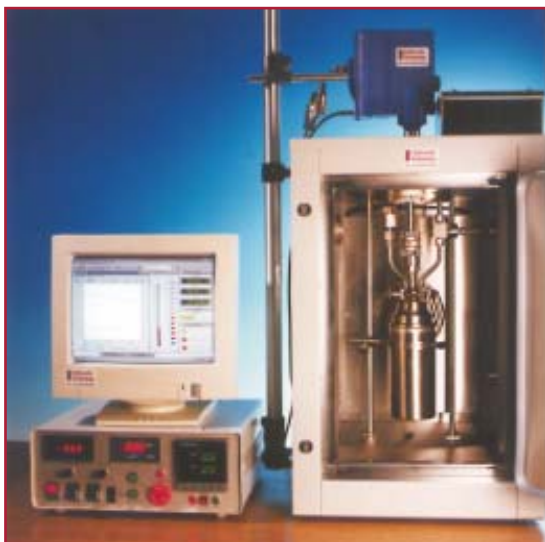
- Assessment of the integrity of any safety-related interlocks on which safety is being based; together with any other basis of safety provisions.
- Identification of the most appropriate basis of safety for the operation.
- Where emergency relief systems will form the ultimate basis of safety, assessment of the characteristics of the reaction system (e.g. tempered or gassy). This will involve evaluation of the consequences of the worst credible scenario(s) identified in Phase 2. This will utilise adiabatic calorimetry to simulate the scenario(s) to obtain the necessary data.
- Preliminary relief system sizing calculations (based on DIERS methods, but using available data from Phases 1 & 2) for two-phase homogeneous flow to indicate whether the existing relief system is clearly adequate (or inadequate).

### Decision

Does the data indicate a sufficient margin of safety between the existing relief size and the short form calculated size or are more detailed and formal calculations required?

### Full Level

- The preliminary vent sizing calculations will be supplemented with an in-depth DIERS analysis for multi-phase, homogeneous flow. This will include a detailed analysis of vent line restriction effects and relief abatement system sizing.



Adiabatic Pressure Dewar Calorimeter ADCII

## FREQUENTLY ASKED QUESTIONS

**Q. I have a multi-product plant but venting is not my preferred basis of safety. Is PreVent still relevant?**

A. Yes. Whilst the ultimate basis of safety for many exothermic reactions is emergency relief venting, other reactions use an alternative basis of safety. PreVent can be used to assess the adequacy of any basis of safety for any product and reactor combination.

**Q. I rely on safety critical instrumented systems as part of my basis of safety. Would PreVent take account of these?**

A. Yes. The risk assessment (Phase 2) of the PreVent approach will take account of any safety critical instrumented systems. Although the specification, design or verification of Safety Integrity Levels (SIL) according to IEC 61508 & IEC61511 is not part of a PreVent assessment, Chilworth Technology can undertake such studies separately.

**Q. We completed a vent sizing assessment several years ago. Can the design basis be verified using PreVent but without repeating the work that has already been performed?**

A. Yes. A gap analysis using PreVent methodology can be conducted with only missing data being obtained. Any existing data and information can be cost-effectively verified within the remit of a PreVent study.

**Q. I don't have any laboratory data on my processes, but they have been running for many years and I've got plenty of plant experience. Can I use this plant data for the review?**

A. Whilst plant data can offer a valuable understanding of the process, it will seldom be sufficiently quantified to allow detailed calculations to be performed. Equally, it will be describing the normal operating behaviour of the process, and will offer no evidence of the consequences if control upsets occur. So plant data can be incorporated into the study and can short-cut some steps, but additional testing will probably be required.

**Q. I already have a relief system that I'm confident is adequate for everything that I'm handling. Why would I need PreVent?**

A. If you have documented information covering process data, assessment of failure scenarios and vent sizing calculations, for all of your processes, your confidence is justified and you probably don't need to conduct further studies. However, have you assessed your basis of safety in light of process improvements you have made since installing the relief system?

**Q. Environmental pressures are forcing me to reassess my existing venting strategy of relieving to atmosphere. If I just add a treatment system on the end of my existing vents, I don't need to go down the PreVent route do I?**

A. Any change to a relief vent system will have an influence on its operational efficiency. The new arrangements must be re-calculated as a whole using the appropriate runaway reaction data. Indeed, any plant change may have an impact on the potential failure scenario used for vent design, and these should equally be assessed before implementation.

# Process Reaction Evaluation & Vent Assessment (PreVent)

## ADVANTAGES OF PREVENT

Many companies already employ the 3 phase full level strategy for reaction hazard assessment. Normally the procedure is undertaken through formal stages of assessment (similar to the full assessment in PreVent). Within PreVent we introduce the implementation of short-form (or screening) procedures to remove any unnecessary in-depth assessment. If at any stage of a screening study more detailed information is required, the analysis can rapidly and seamlessly enter a "full" level analysis programme. This technique developed by our research team has provided clients with focused and effective solutions and permits a faster and cost-effective mechanism for reaction hazard evaluation, using methods in line with industry best practice.

The PreVent approach permits rapid evaluation of the suitability of existing (or planned) reactors for new processes and allows any required process or plant change requirements to be identified at an early stage in process development. Chilworth Technology has specifically developed simplified forms of the DIERS equations for this purpose. Our engineers apply appropriate safety factors to the calculations to ensure that there is sufficient safety margin on the required relief area. This enables further studies to focus on areas that are more hazardous or require a higher degree of engineering involvement and a longer development timescale.

Should calculations show that the existing relief area is insufficient or just bordering on acceptability we will formulate a more in-depth study of the proposed process and installation, to accurately define the vent size and recommend control measures to ensure that the basis of safety is not breached. This will involve further testing, including such experiments as closed cell adiabatic calorimetry and, potentially, blow-down trials and tempering tests. However at this phase the credible failure case has already been defined and kinetic data for this scenario has already been measured, therefore the extent of further testing is kept to a minimum.

A PreVent study of your processes can provide an early identification of scale-up hazards and confirm plant / reactor suitability when optimising new or existing processes.

### Summary

- Low cost short form screening procedure.
- Rapid evaluation of the suitability of existing reactors to a new process.
- Seamless entry into full level analysis programme if necessary.
- Early identification of scale-up hazards and plant suitability.
- Provides the data you need for DSEAR / CAD compliance work.

For further information, contact Chilworth Technology.



Screening Calorimeter



Reaction Calorimeter (Picture Courtesy of Mettler Toledo)

# P r e V e n t

(Process Reaction Evaluation & Vent Assessment)

## CHILWORTH SERVICES IN PROCESS SAFETY

As well as chemical reaction evaluation we also provide a range of testing and consultancy services to the processing industry, covering:-

- Dust/Gas/Vapour Explosion
- Electrostatic Hazards
- Hazardous Area Classification
- IEC61508/11 SIL Determination
- Chemical Process Optimisation
- Regulatory Testing (NONS, SDS, CHIP, CPL, UN)
- ATEX / DSEAR Audits
- Major Hazards (Seveso II / COMAH)
- HAZOP, Fault Tree
- Incident Investigation / Forensic Engineering / Expert Witness
- Loss Prevention / Risk Management
- Training

For further information and a comprehensive list of the services available, please contact one of our offices detailed below.



Consultancy



Testing to GLP Standard



Training

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