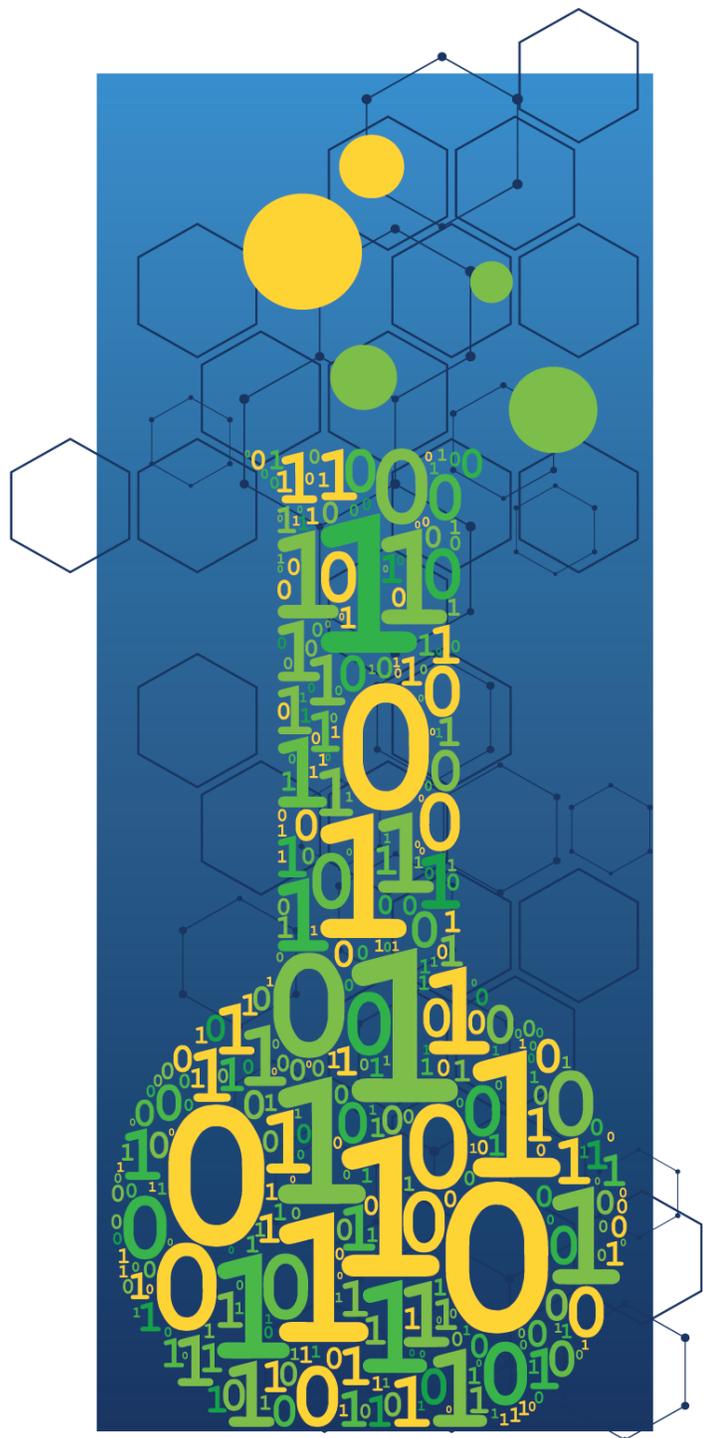


Development of Kinetic Models - Part II. Pressure Relief Systems



An ioMosaic Corporation White Paper

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IO MOSAIC CORPORATION

Development of Kinetic Models - Part II. Pressure Relief Systems

Process Safety and Risk Management Practices

authored by

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August 25, 2022

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1 Introduction

Safe storage, handling, and transportation of reactive chemicals is challenging. Characterization of both desired and undesired chemistries requires a variety of methods including theoretical and computational screening, testing, and detailed modeling [1]. A multitude of process and environmental conditions can influence reaction rates such as contamination, reactant accumulation, loss of agitation, loss of cooling, etc. Identification and characterization of undesired chemistries are often missed at the development stage and/or not communicated properly to toll manufacturers and production facilities during scale-up. Safety data sheets may not be adequate and cannot be solely relied upon for safe storage, handling, or transportation of reactive chemicals. Exothermic runaway reactions can cause loss of containment, significant loss of property and life, and environmental impact [2].

Adiabatic and isothermal calorimetry are often used to characterize chemical reactions. Calorimetry data can then be reduced and used for direct scale-up or to develop simple and detailed chemical reaction kinetic models. Kinetic models are coupled with fluid dynamics for the assessment of thermal stability, process optimization, and pressure relief systems and vent containment design.

Two types of kinetic models can be developed, (a) simple or isoconversion models [3], and (b) detailed models. Isoconversion models are easy to develop, do not require information about stoichiometry, phase change, or vapor/liquid equilibrium, but cannot be used for pressure relief design. They are mostly used for thermal stability assessments where phase change can be neglected and where there is no mass exchange with the system boundaries.

Detailed models require the development of reaction stoichiometry with thermophysical and transport properties. They are mostly used for modeling the dynamics of pressure relief systems and vent containment design, process dynamics, as well as thermal stability assessments. Although they are more complex to develop than isoconversion models, they can be used to extend limited test data to wider ranges of composition, temperature, and pressure. Detailed kinetic models are preferred over direct scale-up methods because they often result in more practical designs and optimal risk reduction.

In this paper we provide an overview of how detailed kinetic models are developed from calorimetry data and how they are used for the modeling pressure relief systems and thermal stability.

2 Direct Scale-up vs. Kinetic Modeling

Direct scale-up methods have been used to develop relief requirements and vent sizing for runaway reactions since the early 1990s. Direct scale-up methods have been popular because one is able to measure in a laboratory test the required relief size in equivalent vent area per unit mass of a reacting mixture, in²/kg, and then scale it up to plant scale equipment.

The primary advantage of the direct scale-up method is its simplicity. The user does not have to provide thermophysical and transport properties or use complex models for relief sizing. However, direct scale up methods have a lot of disadvantages and are not capable of providing all the information for safe and optimal design that is now required by recognized and generally accepted

good engineering practice (RAGAGEP) [4, 5, 6].

Direct scale up methods are only valid at the conditions of the test. This includes but is not limited to fill level, relief set pressure, chemical composition, heating rate, and vapor/liquid disengagement characteristics of the test cell and associated vent. Additional tests have to be conducted if different conditions need to be considered. This can be costly both in resources and schedules.

Direct scale up methods tend to result in overly conservative venting requirements. While this may be considered to be favorable for vessel protection, an oversized vent can cause safety complications for effluent handling and subsequent flammable or toxic dispersion [6]. A bigger vent is not necessarily better.

Kinetic modeling methods for pressure relief couple detailed chemical reaction models with fluid dynamics to develop the required vent size. These methods have also been in use since the early 1990s when the American Institute of Chemical Engineers (AIChE) initially developed the computer program SAFIRE [7] through its Design Institute for Emergency Relief Systems (DIERS). SAFIRE was later replaced with SuperChemsTM for DIERS¹ by Arthur D. Little Inc. under a contract to AIChE DIERS.

Kinetic modeling methods for pressure relief systems are highly recommended because of their inherent advantages over direct scale-up methods [8]. A disadvantage of the kinetic modeling methods is the availability of suitable detailed chemical reaction models, stoichiometry, thermophysical and transport properties to couple with fluid dynamics models. Fortunately, the development of detailed chemical reaction models has become much more practical over the years as discussed below. Detailed chemical reaction models can be developed quickly and cost effectively using a combination of adiabatic calorimetry testing and advanced computational tools.

Once a detailed kinetic model is developed, it can be used over and over again in many process design and modeling applications.

3 Detailed Chemical Reaction Models

Only detailed models are recommended for use with pressure relief systems and vent containment dynamics. Detailed models require the development of reaction stoichiometry in addition to reaction rates. Representative reaction stoichiometry is a must because it is necessary for development of chemical compositions as the reaction proceeds. Chemical compositions drive the vapor/liquid equilibrium conditions and as a result, the fundamental pressure-temperature relationship of the system. This in turn determines the coincident temperature and reaction rate(s) at the opening pressure of the relief device and the effective molecular weight and volumetric flow rate of what is being vented. Simple or isoconversion reaction models cannot be used for the evaluation or design of pressure relief requirements.

Development of detailed kinetic models requires the dynamic simulation of the test cell and the time-dependent mass and energy balances as well as the pressure-volume-temperature (PVT) and vapor-liquid-equilibrium (VLE) behaviors. The accelerating rate calorimeter (ARCTM), the auto-

¹SuperChems is a trademark of ioMosaic Corporation

matic pressure tracking adiabatic calorimeter ² (APTACTM), the vent sizing package ³ (VSP2TM), and Phi-TEC IITM are widely used ⁴ for the measurement of reaction data to develop such models. SuperChems ExpertTM is the method of choice to simulate the calorimetry tests to develop the detailed models. SuperChems Expert can model detailed vessel dynamics with multiple multiphase reactions and can handle special cases such as liquid full cases and retrograde and phase change as the reactions proceed and as the mixture changes composition due to reactions.

4 Reaction Stoichiometry

The development of reaction stoichiometry and rates requires expert skills [8] and some understanding of the chemistry involved. Use of chemical equilibrium tools such as those provided in SuperChems Expert can speed up the development of reaction models. In general, the initial reaction rate estimates are provided using simple kinetic models [3].

It is important to establish the correct stoichiometry of chemical reactions in order to develop adequate pressure relief requirements and to select effective vent containment strategies. The stoichiometry of a chemical reaction significantly influences the system pressure-temperature relationship and/or physical equilibria during venting. The set pressure or opening pressure of a relief device will correspond to a coincident temperature which in turns corresponds to a specific reaction rate. If we assume that reaction rates typically double every ten degrees, then special care must be exercised when characterizing the system pressure-temperature. Erroneous characterization of the system pressure-temperature relationship can yield a significantly undersized pressure relief device or a significantly oversized pressure relief device. Either situation can lead to unsafe conditions.

Vapor/liquid equilibrium is heavily dependent on reaction stoichiometry since the stoichiometry defines what chemical species can be present at specific pressure and temperature conditions. The chemical species physical, thermodynamic, transport, environmental, toxicity, and flammable properties influence most aspects of pressure relief design, safe storage and handling, as well as safe discharge [6], and a multitude of regulatory compliance requirements. The volumetric discharge rates during relief depend on the vapor quality of what is being vented as well as the chemical molecular weights, densities, and other thermodynamic properties such as enthalpy and latent heat. These are amongst the many reasons for why isoconversion models cannot be used to develop relief requirements, especially for runaway reactions where single or multiphase flow can occur.

5 Constrained Gibbs Free Energy Minimization

Despite the fact that we are mostly concerned about major species that can influence the venting rates and energy balances during a runaway reaction, it is not sufficient to simply assume an arbitrary type of a chemical product with arbitrary thermophysical and transport properties. It

²ARC and APTAC are trademarks of Netzsch

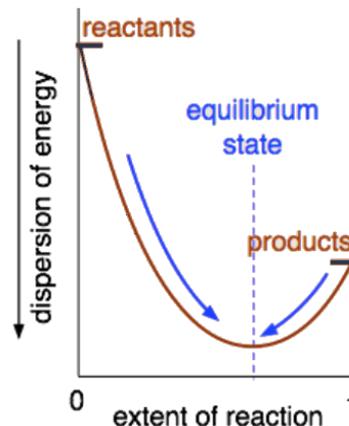
³VSP2 is a trademark of Fauske and Associates LLC.

⁴Phi-TEC II is a trademark of H.E.L Group

is possible to establish the identity of some reaction products using analytical methods such as gas or liquid chromatography or mass spectrometry (GC/MS) at various stages during adiabatic calorimetry testing. It is often preferred to take samples for GC/MS analysis at the end of a test in order to reduce complexity and testing costs. This type of analysis is very helpful but is often not sufficient to develop the entire stoichiometry. In some systems, the stoichiometry may also vary with pressure and temperature during a runaway reaction.

We can use multiphase Gibbs free energy minimization [9] to develop reaction stoichiometry via simultaneous physical and chemical equilibrium. Chemical reactions that are thermodynamically possible and that are fast (combustion reactions) will typically be well represented with an equilibrium state or end point.

A reaction that is thermodynamically possible but lacks a fast mechanism (rate or mixing limited liquid reaction) is said to be kinetically limited. Some measurements are required to constrain the equilibrium calculations. The following assumptions are implicit in this methodology [8]:



1. Slow reactions are the passive constraints that will retard the relaxation of the system from reaching complete equilibrium,
2. Fast reactions will equilibrate the system subject to the constraints imposed by the slow reactions, and
3. The system will proceed to its final state through a sequence of constrained equilibrium states at a rate controlled by the slow reaction steps.

We note that for a reversible chemical reaction, the ratio of forward to reverse kinetic rate is equal to the equilibrium constant, where the equilibrium constant is calculated entirely based on thermochemistry.

$$\frac{k_f}{k_r} = k_{eq} \quad (1)$$

where k_f and k_r are the forward and reverse kinetic rates and k_{eq} is the equilibrium constant. Numerous factors can influence the direction of a reversible chemical reaction.

We can constrain the Gibbs free energy minimization to yield a restricted equilibrium state or a restricted conversion of one or more chemical reactions or chemicals [8]. The constraints can be obtained from measured calorimetry data, and/or measured GC/MS chemical identity or composition data.

A constraint that is commonly used involves the final pressure observed after cool down of a closed adiabatic calorimetry test, i.e. the total ratio of non-condensable gas production or number of moles to the total number of moles. Another common constraint that can be used is the molar ratio of selected species as identified by a GC/MS for example at the end of the reaction or during

Table 1: Constrained Gibbs free energy minimization data for di-t-butyl peroxide system [8]

	Case 1	Case 2	Case 3
Atom and Constraints Matrix rank	5	6	9
Maximum number of independent reactions	96	95	92
Scaled Gibbs free energy	1232	1242	1564
Initial temperature (K)	383	383	383
Final temperature (K)	463	463	463
Initial pressure (Pa)	275000	275000	275000
Final pressure (Pa)	3290000	3290000	3290000
Initial number of moles (kmol)	254.815	254.815	254.815
Final number of moles (kmol)	277.98658	281.616	267.5
Change in number of moles (kmol)	23.17158	26.801	12.685
Initial volume (m3)	10.4	10.4	10.4
Final volume (m3)	51.6	46.8	10.8
Volume change (m3)	41.2	36.4	0.362
Initial enthalpy (MJ)	87000	87000	87000
Final enthalpy (MJ)	86400	86600	86900
Enthalpy change (MJ)	-516	-388	-69

the reaction. A measured heat of reaction can also be used as a constraint. SuperChems Expert version 11.0 provides the user several options to constrain multiphase direct minimization of the Gibbs free energy.

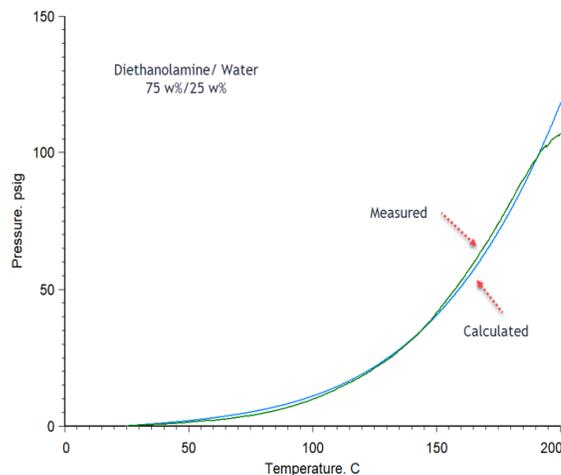
An example of using such constraints to develop the stoichiometry of di-t-butyl peroxide decomposition is illustrated in Table 1. Reference [8] includes two detailed examples where constrained minimization of the Gibbs free energy is used to develop the stoichiometry for di-t-butyl peroxide decomposition and methanol/acetic acid esterification.

The additional constraints can either be equality or inequality constraints. The equality constraints are added to the atom matrix constraints while the inequality constraints are typically added separately. SuperChems Expert also uses additional inequality constraints for phase stability. When a user defines a mixture in SuperChems Expert, the atom matrix is automatically created and the user is provided with an option to add equality and inequality constraints for four phases (solid, vapor, liquid I, liquid II). The Gibbs constrained multiphase equilibrium method assumes that the user can select a large listing of potential reaction products candidates from the SuperChems Expert database and that all those products have the required thermophysical properties. The SuperChems Expert properties databanks include approximately 3000 chemicals. SuperChems Expert also includes property estimation and group contribution methods where the user can add new chemicals for use in dynamic simulations or in the minimization of the Gibbs free energy method.

6 Vapor-Liquid Equilibrium

The nonideal behavior of a reacting chemical mixture can have a substantial impact on the pressure-temperature relationship of the reaction system. In addition to influencing compositions in the vapor and condensed phases, nonideal behavior also influences other thermodynamic and transport properties such as internal energy, heat capacities, densities, liquid isothermal compressibility, thermal conductivity, viscosity, etc.

During a chemical reaction mass is conserved but reacting species are converted into different product species. This makes modeling of the vapor/liquid equilibrium more challenging. In reality, the phase envelope of the reaction mixture is changing over time as the reaction is taking place. One of the many advantages of using closed volume adiabatic calorimetry centers around the pressure-temperature data measured before the onset of a chemical reaction is detected. This data is valuable because it can be used to verify the vapor/liquid behavior of the reactants and/or to develop missing reacting mixture component properties as shown in the Figure to the right for the binary system diethyl amine and water.



Adiabatic calorimetry can be used to develop the vapor pressure curve of a pure component, or in the case of the binary system diethyl amine and water, to determine the binary interaction parameters (BIPs) of a mixture. This is accomplished by simulating the adiabatic calorimetry test using SuperChems Expert and finding the best estimate of BIPs. For measurement of the vapor pressure of a single component, the adiabatic calorimetry test is often conducted by initially pulling a vacuum on the vapor space or by using an inert gas, such as helium, with low solubility in the liquid phase. The vapor pressure can be established by subtracting out the contribution of the inert gas from the measured vapor pressure. For many single components that do not decompose, the adiabatic calorimetry can also be used to determine the critical point. Note that vapor pressure measurements are subject to the accuracy limits of the pressure transducer used in the adiabatic calorimeter. A vapor pressure curve can be used to establish the normal boiling point as well as the latent heat of vaporization.

SuperChems Expert uses an equation of state with modified mixing and combining rules to model phase and chemical equilibria and thermophysical properties. It is not uncommon for adiabatic calorimetry tests to reach high pressures (≥ 2000 psig) and high temperatures (≈ 400 °C) where solubility effects and vessel metal stretch can become important. Reaction systems can also exhibit supercritical behavior and heat of dilution/mixing effects. Therefore, the use of an accurate equation of state is a must for the modeling of calorimetry data. We note that SuperChems Expert also includes detailed methods for the calculation of formation energies as a function of temperature. Heats of reaction (positive or negative) as well as solution effects are implicitly realized as conversion occurs for one or more chemical reactions.

7 Developing Detailed Reaction Models

The development of reaction models suitable for pressure relief systems design or evaluation requires experience and the availability of software tools such as SuperChems Expert to dynamically simulate the reaction calorimetry test.

The simulation should start at the beginning of the test well before any reaction takes place. Small amounts of non-condensable gas generation and/or small temperature deviations can have a significant impact on pressure-temperature behavior of the system. First, simulate the calorimetry test without a reaction to confirm the reactants thermophysical properties and vapor-liquid equilibrium behavior. Then a kinetic expression is developed using simple methods and used as a starting point for the dynamic simulation.

In order to develop a valid kinetic model, five indicators must be demonstrated to have good fits as shown in Figures 1 and 2:

1. Temperature vs. time: This should include the heat-wait-search portion of the calorimetry test or the constant heat ramp portion of the test.
2. Pressure vs. time: This should include the heat-wait-search portion of the calorimetry test or the constant heat ramp portion of the test.
3. Pressure vs. temperature: This is a critical system curve because it establishes the reaction rate at the opening pressure of a relief device. This relationship is sometimes intentionally biased to be slightly conservative to account for uncertainties in testing methods and thermophysical properties.
4. $\frac{dT}{dt}$ vs. time: This is used to also show the goodness of fit for the cool down portion of the test. Often, a logarithmic plot of $\frac{dT}{dt}$ vs. Temperature is used.
5. $\frac{dP}{dt}$ vs. time: This is used to also show the goodness of fit for the cool down portion of the test. A logarithmic plot of $\frac{dP}{dt}$ vs. Temperature or $\frac{dP}{dt}$ vs. $\frac{dT}{dt}$ is also used.

The simulation should also include the calorimetry test cool down portion to confirm that the right amounts of non-condensable gas are reflected by the kinetic model. The drift portions of the test should also be replicated by the dynamic simulations as shown in Figure 1. In general, it is preferred to demonstrate the performance of the kinetic model against additional test data.

For complex reaction systems, the reactions have to be decoupled and fit in sequence. This can be tedious and can require a lot of effort for very complex chemistries where multiple reactions are taking place. Kinetic models are used to extend the use of the measured data over wide temperature, pressure, and composition ranges and conditions. Less effort is typically required for single molecule decompositions or polymerization reactions.

Figure 1: Best fit kinetic model developed using SuperChems Expert for the decomposition of 50 % dicumyl peroxide in toluene

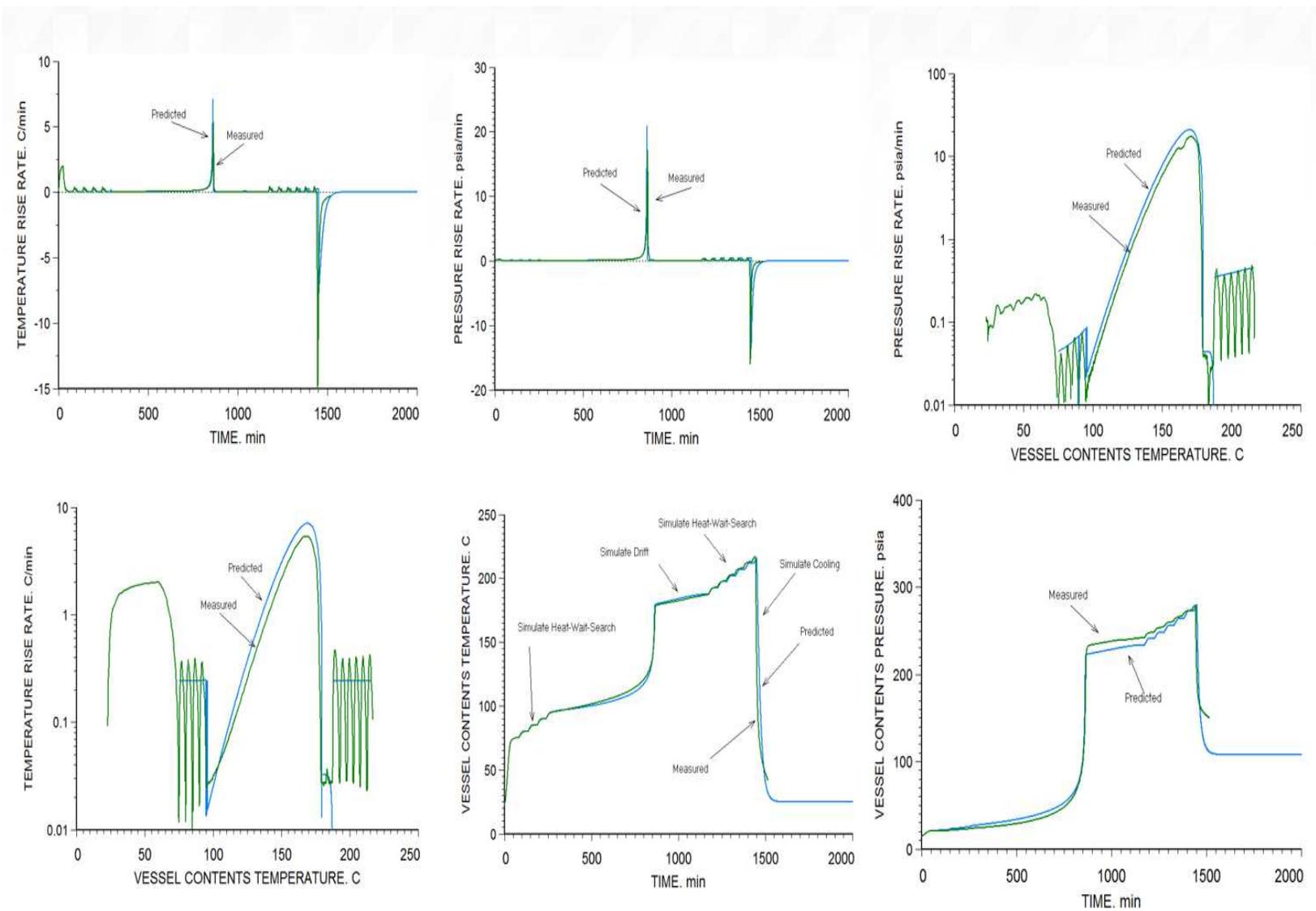
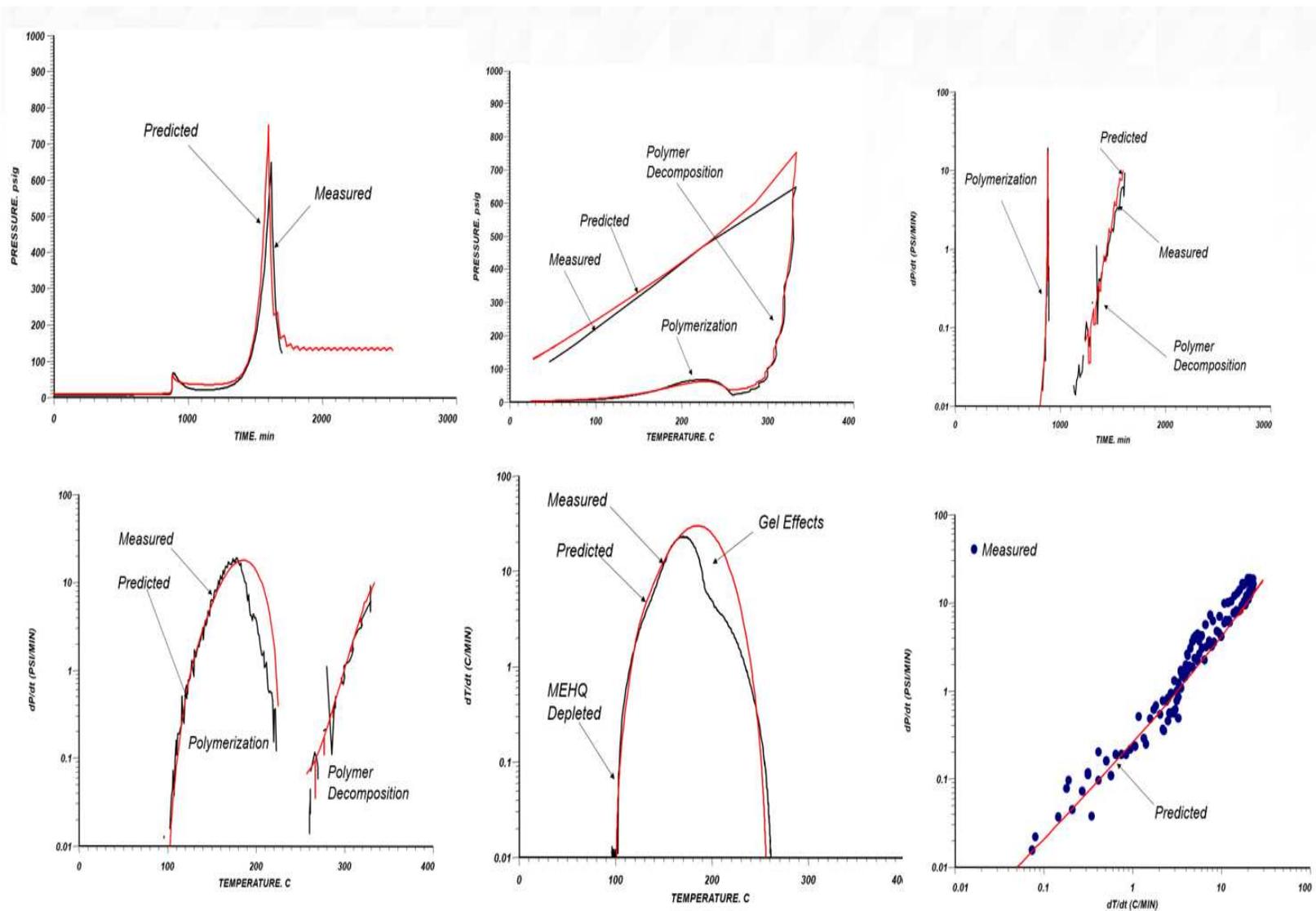
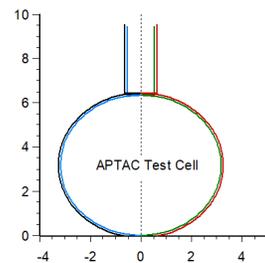


Figure 2: Best fit kinetic model developed for the polymerization (and polymer decomposition) of butyl acrylate inhibited with MEHQ



8 Adiabatic Calorimeters

Some of the most popular calorimeters used for measuring reaction data include the accelerating rate calorimeter (ARC), the automatic pressure tracking adiabatic calorimeter (APTAC), and the vent sizing package (VSP2). The APTAC and VSP2 use pressure balancing to reduce the thermal inertia, ϕ , of the system while the ARC does not. The ARC is widely used because of its simplicity, adiabaticity, detection sensitivity, and tracking capabilities. The ARC, APTAC, and VSP2 cannot be used to measure endothermic heats of reaction.



Thermal inertia values as low as 1.15 can be achieved in the APTAC and VSP2. Low thermal inertia test data is often desired because it is more directly applicable for plant scale vessels. However, high thermal inertia tests are just as useful and can be instrumental to capture highly energetic reactions in their entirety. In general, a combination of low and high thermal inertia tests should be provided to ensure that intermediate reactions are not being masked by thermal inertia effects. High thermal inertia data can be easily corrected to plant scale low thermal inertia using detailed modeling software like SuperChems Expert .

Despite the use of a variety of heating elements and insulation to minimize heat loss due to conduction, convection, and reflux condensing, the measured heat of reaction can be underestimated in some unique cases by up to 20 %.

The APTAC and VSP2 can also be used to perform vented calorimetry tests. Vented tests are useful for direct scale-up of relief requirements and the assessment of venting regimes and foaming tendencies of reacting mixtures. It is preferred, where practical, to develop the reaction kinetic model using closed test cell data and to validate such models using vented calorimetry test data.

Typical adiabatic calorimeter test cell volumes range from 8 to 130 ml as shown in Table 2. Test cells are available in varying materials of construction including glass, stainless steel, titanium, hastelloy, and tantalum.

9 Using Detailed Models in Pressure Relief Systems Design

The kinetic model developed for butyl acrylate polymerization and polymer decomposition [10, 11, 12, 13] (see Figure 2) was used to evaluate the relief requirements for a large butyl acrylate storage tank under fire exposure without fire proof insulation or fixed water sprays. The tank has a total volume of 29,000 gal and is normally 92 % full (200,000 lbs). The tank has a design pressure of 150 psig and a design temperature of 150 F. Initially the contents are at 74 F and 0 psig. The tank vents to the atmosphere via an 18 inch rupture disk set at 15 psig.

The contents are typically inhibited with MEHQ. Extended storage durations can deplete the inhibitor. Two simulations were conducted using SuperChems Expert to study the impact of fire exposure on relief requirements. The results are shown in Figure 3 for starting conditions of 1 PPM of MEHQ at initial fill levels of 50 % and 92 %.

Table 2: Typical adiabatic calorimeter test cell volume and mass data

Test-Cell Name	Material of Construction	Mass [†] g	Volume [‡] at 25 °C ml	Specific Heat J/kg/°C	Specific Heat cal/g/°C
ARC	Stainless Steel 316	17.64	9.5497	452.5	0.1082
APTAC	Titanium	33	136.4	519.7	0.1242
APTAC	Titanium	55	136.4	519.7	0.1242
APTAC	Hastelloy C	118	136.4	365	0.0872
APTAC	Stainless Steel 316	94	136.4	452.5	0.1082
VSP2	Stainless Steel 304	24.9	110.7	469.2	0.1121
VSP2	Stainless Steel 316	24.8	110.7	452.5	0.1082
VSP2	Hastelloy C-276	28	110.7	365	0.0872
VSP2	Titanium	14	110.7	519.7	0.1242

[†] In some cases, the fittings mass should also be added to the thermal inertia.

[‡] Test cell volumes should include the additional volume of tubing and valve(s). For ARC this can be equivalent to 0.48 ml approximately.

As shown by Figure 3 the tank becomes liquid full due to thermal expansion of the liquid at 92 % initial fill level. The rupture disk opens as a result and venting continues at near atmospheric conditions until the reaction rates become high enough to raise the pressure to approximately 80 psig.

This illustration is but a simple example of what can be accomplished when good kinetic models are coupled with detailed fluid dynamics. The simulations enable the user to evaluate many what-if scenarios, to determine the dynamic reaction force loads caused by the rupture disk opening, and to determine the vapor quality and mass flow rate during venting, etc. More detailed dynamics can also be performed [14, 4, 5] to study available pre- or post- release mitigation measures including but not limited to the use of quench fluid, more inhibitor injection, fire proof insulation, fixed water sprays, estimated time to failure, estimated time to yield, safe discharge location, etc.

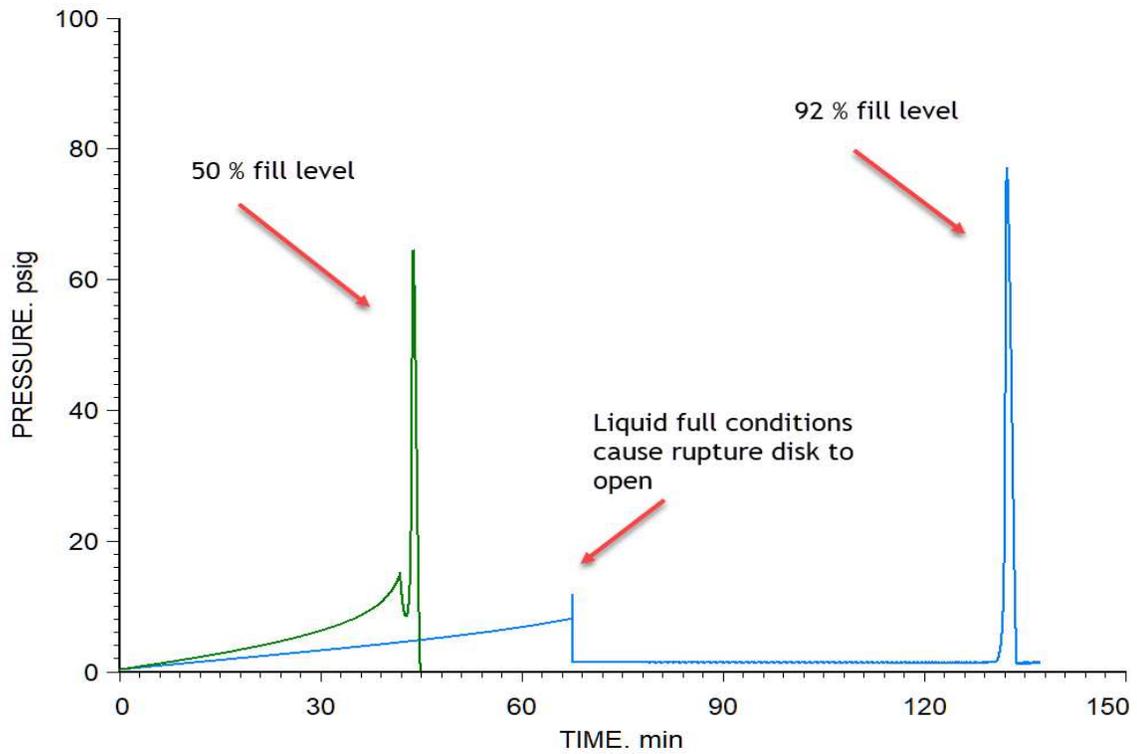
When planning modifications to existing equipment or developing new designs, kinetic modeling for pressure relief design is almost always more cost effective and yields optimal risk reduction.

10 Conclusions

We have outlined a proven and systematic process for the development of detailed chemical reaction kinetic models. This systematic process uses some of the advanced computational tools available in SuperChems Expert with limited adiabatic calorimetry test data.

Detailed kinetic models developed using this process can be coupled with fluid dynamics to establish practical relief requirements and for thermal stability assessment. Kinetic modeling methods are highly recommended for pressure relief systems design because of their flexibility, optimal risk reduction, and their inherent advantages over direct scale-up methods. Once a detailed ki-

Figure 3: Calculated pressure-time histories for fire induced butyl acrylate runaway polymerization using SuperChems Expert



netic model is developed, it can be used over and over again in many process design and modeling applications.

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About the Author



Dr. Melhem is an internationally known pressure relief and flare systems, chemical reaction systems, process safety, and risk analysis expert. In this regard he has provided consulting, design services, expert testimony, incident investigation, and incident reconstruction for a large number of clients. Since 1988, he has conducted and participated in numerous studies focused on the risks associated with process industries fixed facilities, facility siting, business interruption, and transportation.

Prior to founding ioMosaic Corporation, Dr. Melhem was president of Pyxsys Corporation; a technology subsidiary of Arthur D. Little Inc. Prior to Pyxsys and during his twelve years tenure at Arthur D. Little, Dr. Melhem was a vice president of Arthur D. Little and managing director of its Global Safety and Risk Management Practice and Process Safety and Reaction Engineering Laboratories.

Dr. Melhem holds a Ph.D. and an M.S. in Chemical Engineering, as well as a B.S. in Chemical Engineering with a minor in Industrial Engineering, all from Northeastern University. In addition, he has completed executive training in the areas of Finance and Strategic Sales Management at the Harvard Business School. Dr. Melhem is a Fellow of the American Institute of Chemical Engineers (AIChE) and Vice Chair of the AIChE Design Institute for Emergency Relief Systems (DiERS).

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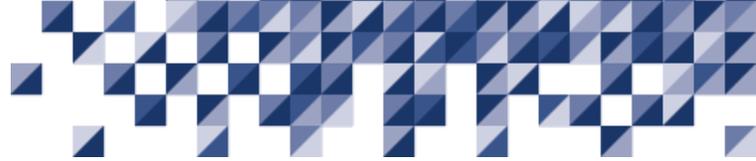
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As a certified ISO 9001:2015 Quality Management System (QMS) company, ioMosaic offers integrated process safety and risk management services to help you manage and reduce episodic risk. Because when safety, efficiency, and compliance are improved, you can sleep better at night. Our extensive expertise allows us the flexibility, resources, and capabilities to determine what you need to reduce and manage episodic risk, maintain compliance, and prevent injuries and catastrophic incidents.

Our mission is to help you protect your people, plant, stakeholder value, and our planet.

Consulting Services

- Asset Integrity
- Auditing and Due Diligence
- Combustible Dust Hazard Analysis and Testing
- Facility Siting
- Fault Tree/SIL/SIS Analysis
- Fire and Explosion Dynamics
- Incident Investigation, Litigation Support and Expert Testimony
- Liquefied Natural Gas Safety
- Pipeline Safety
- Process Engineering Design and Support
- Process Hazards Analysis (PHA)
- Process Safety Management (PSM)
- Reactive Chemicals Evaluation and Testing
- Relief and Flare Systems Design and Evaluations
- Risk Management Program Development
- Quantitative Risk Assessments (QRA)
- Software Solutions
- Structural Dynamics
- Training

Laboratory Testing Services (ISO accredited)

- Chemical Reactivity
- Battery Safety
- Combustible Dust
- Specialized Testing