Process Safety News

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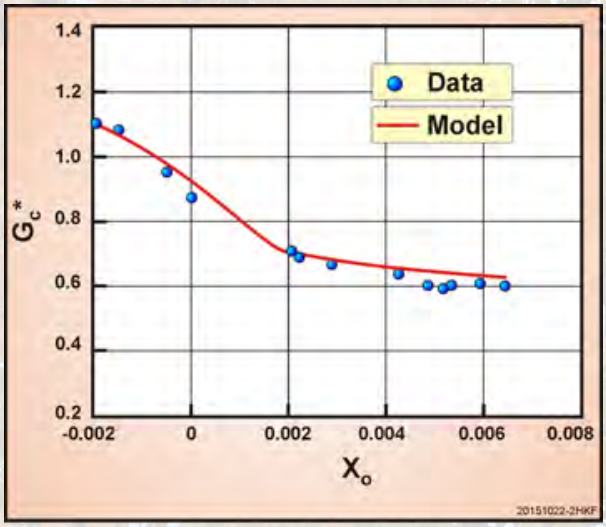
Replacing Complex Two-Fluid Models With a Simple Model That Has No Adjustable Parameters and That is Agreeable With Experimental Data Including Both Non-Equilibrium and Equilibrium Flashing Flows

By: Hans K. Fauske, D. Sc., Regent Advisor, Fauske & Associates, LLC (FAI)

In contrast to the two-fluid models that require numerous assumptions and the corresponding closure equations, the Simple Model can be stated as

$$G = \left[G_{SC}^2 + \left(\frac{1-Y}{G_0^2} + \frac{Y}{G_1^2} \right)^{-1} \right]^{1/2} \qquad (1)$$

where G (kg m^{-2} s^{-1}) is the Non-Equilibrium or Equilibrium two-phase flow rate including the effects of subcooling (G_{SC}), Y is the dimensionless independent variable ranging from 0 to 1 and G_0 and G_1 are the corresponding asymptotic flow rate limits. For all specified stagnation conditions (subcooled liquid, saturated liquid and liquid-vapor mixtures) and flow geometries (nozzle, short and long), the easy to estimate G values in the region between the known asymptotic limits with no arbitrary adjustable parameters are in remarkable agreement with available experimental data. The nozzle constant area length L is the key parameter and values (Y) leading to non-equilibrium and equilibrium flashing flows is provided by (Fauske, 1985, 2017).



Sozzi and Sutherland Nozzle No. 2 Data D = 12.7 mm
Water, P_o = 62 bar, L/D =1.

An example is illustrated below the agreement of the simple model is consistently good for all inlet quality (X_o) conditions, where G_c^* is the dimensionless mass flux, defined as $G/\sqrt{P_o \rho_o}$, and quoting Sozzi and Sutherland (1975), stagnation quality (X_o) in the vessel upstream of the nozzle is based on the density (ρ) in the vessel and the stagnation pressure (P_o):

$$X_o = \frac{1/\rho - v_f(P_o)}{v_{fg}(P_o)} \qquad (2)$$

when the liquid is subcooled, $v_f > 1/\rho$ and, consequently Eq. 2 results in $X_o < 0$ as a negative quality.

It should be noted that the short nozzle No. 2 (D = 12.7 mm and L/D = 1) non-equilibrium data by Sozzi and Sutherland (1975) have provided difficulties in predicting especially with two-fluid modelling which required empirical adjustment to fit the test results (Levy, 1993).

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Dr. Hans K. Fauske is an original founding partner of Fauske & Associates, LLC and currently serves as Regent Advisor

Letter From the President

Life is hectic, and time is precious. As both a father and president of a thriving business, I know this all too well. It seems like there is always somewhere I need to be and some project I need to address, but not surprisingly, the schedules for all the various commitments in my life don't always mesh together in a convenient manner. That is why I appreciate when I am able to identify a way to make the most of my time and accomplish multiple tasks at once.

With this in mind, at Fauske & Associates, LLC, (FAI) we are pleased to offer our customers a single resource for dust testing, consulting, engineering and training – all functions critical to the development of an effective combustible dust process safety program.

We recognize that your time is valuable. By offering all of these services in one place, our experts are able to provide expert and efficient end-to-end assistance that considers all the pieces of your intricate safety puzzle, both individually and as a whole, in order to help you achieve optimum results.

We know you have many places that you can turn for support in building and maintaining your safety programs, and are grateful you have chosen us.

Check out our website at http://www.fauske.com/chemical-industrial/testing/combustible-dust or email us at dust@fauske.com to learn more about how we can assist you with your combustible dust needs.

Stay safe this fall!

H. Kristian Fauske
President

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Statement of Purpose:

FAI's "Process Safety News" is intended to be a forum on recent advances in chemical process safety and FAI's current and related offerings in this area. It will address subscriber's concerns regarding issues and practices for relief system design as well as laboratory testing and techniques for process safety management.

Inquiries:

FAI's "Process Safety News" is published by
Fauske & Associates, LLC
16W070 83rd Street, Burr Ridge, IL 60527
Toll Free: 877 FAUSKE1, +1-630-323-8750
Fax: +1-630-986-5481
info@fauske.com www.fauske.com

Executive Director

H. Kristian Fauske

Art Director

Sara Peters

Contributors

David Dale
AnnMarie Fauske
Dr. Hans K. Fauske
Kris Fauske
T.J. Frawley
Arturo Garza
Jeff Griffin
Lisa Karcz
Dr. Donald Knoechel
Sara Peters
Carol Raines
Gabe Wood
Mark Yukich

Publisher

Fauske & Associates, LLC

FAUSKE & ASSOCIATES, LLC FINALIZES PARTNERSHIP AGREEMENT WITH THE UNIVERSIDAD AUTONOMA DE NUEVO LEON (UANL)

By: Arturo Garza, Owner/Founder BDSI, Fauske & Associates, LLC Agent in Mexico

UANL is the State University of Nuevo León, which is home to more than 200 industries, several of which are among the most important in Mexico: Alfa, Femsa, Cemex, Gruma, Ternium, Deacero, Xignux, Cydsa, Vitro, Banorte, Afirme, Soriana, to name a few. These are involved in activities such as: aluminium, autoparts, petrochemicals, synthetic fibers, food and drinks, corn flour, steel, cement, glass, power generators and transformers, banking, insurance, and department store retail. Newcomers in the industry of the State include: biotechnology, renewable energy, mechatronics, aeronautics.

Resulting from NAFTA, very rapid growth has been registered in the automotive and autoparts sector. Nuevo León has grown to become the third largest producer in the country, with a share of approximately 27% of total output.

UANL is the third largest public University in Mexico, with seven campuses, 26 higher education departments and 38 R&D centers. It has an outstanding record of close collaboration with Industry. For example, the University has "partnered" with large companies like Whirlpool and others to perform R&D.

For this, the Center for Social and Business Linkage was created with the main objective to combine efforts and capacities to carry out tasks of common interest, through the different University units. Also, throughthe execution of scientific, technological, productive, academic, and cultural activities that contribute to social and business development, as well as the integral formation of students and teachers that transform their actions into direct benefits for society.

Currently, UANL is working with industry on projects that seek to solve problems relating to manufacturing, metallurgy, natural gas, electricity, electronics, software, health, biotechnology, automotive sector, among others.

The General Agreement signed sets the stage for specific collaborative efforts between FAI and UANL. The initial purpose of the partnership is to raise awareness regarding process safety among students and alumni of the school. The next step is to develop a process safety center of excellence that provides support to companies across Mexico and Latin America. The first step will be accomplished by training UANL technical leaders in the discipline of reaction hazards, specifically, how to perform reaction screening using FAI's Advanced Reactive System Screening Tool (ARSST) alongside other instruments. The ARSST will be situated in a laboratory at UANL's state of the art facility in Monterrey, Mexico. This facility is close to the international airport in Monterrey, which makes it easily accessible. FAI and UANL look forward to providing process safety testing and consulting services to local industry.

Awareness of process safety, although present in Mexican industry, is an issue that has yet to be further established, in order to assign it due importance as part of best manufacturing practice, over and above regulation compliance. The aim of this General Agreement is to increase awareness on process safety in Mexican industry via the inclusion of specific courses in the undergraduate and graduate syllabi, research work to be done hand-in-hand with industry, and the provision of services that may generate earnings.

Contact Jeff Griffin, Director, Global Business Development & Strategy at FAI at 630-887-5278 or griffin@fauske.com to learn more.

Arturo Garza Eckermann is owner/founder of Buró de Servicios Internacionales SC (BDSI) and represents FAI as our agent in Mexico

EFFECTS OF TEMPERATURE ON THE LOC OF DIMETHYL SULFOXIDE WHEN MIXED WITH A HIGHER VAPOR PRESSURE SOLVENT

By: T.J. Frawley, Flammability Project and Lab Manager, Fauske & Associates, LLC

Dimethyl Sulfoxide (DMSO) is an extremely versatile solvent with uses spread across multiple industries. It is a by-product of the wood industry, has many uses in the medical field (although some uses are controversial), is an effective solvent due its high solubility, and can be used as a reaction solvent in manufacturing (DMSO.com).

DMSO's effectiveness is partially due to the relatively nonvolatile nature of the substance when compared to other solvents. It has a high boiling point of 189°C and a low vapor pressure. The vapors are quite dense, with a vapor density of 2.70. Air has a vapor density of 1.0. The combination of dense vapors and low vapor pressure contribute to its, again, relatively high flash point temperature of 87°C.

Solvent	Flash Point (°C)
Dimethyl Sulfuroxide	87
Acetone	-18
Tetrahyrofluran	-17
Ethanol	13
Dimethylformanide	58

From a process safety standpoint, as long as the process is ran below the 87°C with DMSO alone, there is little risk. However, once another solvent with a lower flash point is mixed with DMSO, the flash point of that mixture will drop below 87°C, creating an explosive environment. If the process requires higher temperatures and high pressures, the danger increases with additional each degree and millibar.

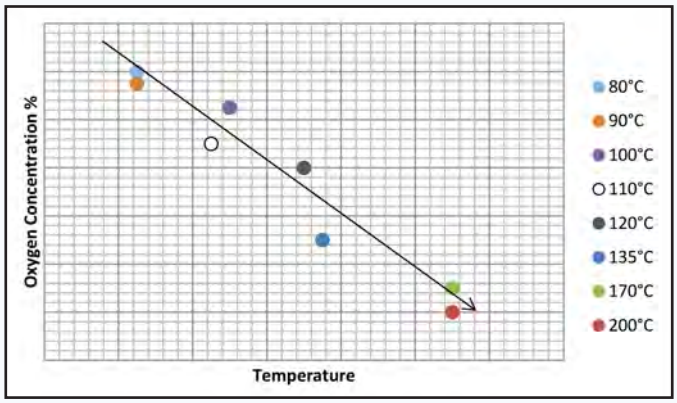
If you are reading this newsletter, I feel safe in assuming that you are aware of the fire triangle and the hazards that exist working with the boundaries of that three-corners geometric shape of fire and fury. Before you think to mitigate the hazard through vent sizing or any other method, let us discuss prevention.

Your product is fuel . Cannot eliminate that leg of the triangle. And while you can attempt to reduce the exposure of your process to an ignition source, it is near impossible to eliminate every single, minute, possible, feasible, conceptual, source of ignition.

This leaves our final leg of the triangle, Oxygen. Here is where the Limiting Oxygen Concentration (LOC) test comes into play. If the process is anaerobic, you can completely inert your process with Nitrogen or Argon. This can get expensive as Nitrogen is not cheap, Argon less so. So you perform an LOC test to determine the lowest percentage of oxygen needed to sustain flammable propagation. And you run your process beneath that number. You are now on the off ramp exiting the danger zone.

But engineer beware. As the temperature increases, the amount of Oxygen needed to propagate an ignition decreases.

Assuming at 1:1 ratio mixture by volume of DMSO and another solvent with a flash point lower DMSO, the LOC of the mixture will decrease as the temperature increases. At lower temperatures the partial pressure of the mixture's vapors will consist mostly of the other solvent. Not enough of the DMSO has vaporized to propagate an ignition in environments that are starved of oxygen. For example, say Sample A has an LOC of 10% O_2 at 14.7 psia at 100°C and DMSO has an LOC of 6.5% O_2 at 14.7 psia at 100°C. The LOC of the mixture of Sample A and DMSO will be closer to 10% O_2 because the partial pressure will consist of a greater percentage of the less dense vapors of Sample A.



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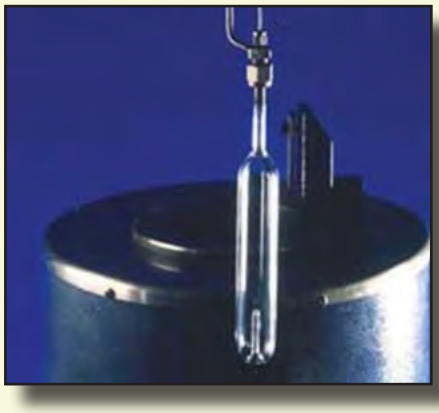
PRE-CARIUS? CARIUS TUBE TESTING FOR HAZARDOUS MATERIALS AND REACTIONS

By: David Dale, Process Safety Manager, Scientific & Medical Products Limited and Jeff Griffin, Director, Global Business Development & Strategy, Fauske & Associates, LLC



The Carius tube apparatus is an old-school device used to thermally test materials on a small scale. The technology is particularly helpful for understanding potentially hazardous reactions or materials. While other tools like the Differential Scanning Calorimeter (DSC) or Advanced Reactive System Screening Tool (ARSST) are good for screening potentially hazardous reactions and providing more robust data, the Carius tube apparatus still has its place in the process safety assessors armory.

When we say the device is 'old-school' – we mean it. The Carius tube was invented by Georg Ludwig Carius in the late 1800's. Compare this to other screening / kinetic evaluation tools like the DSC, invented by Watson and O'Neil in 1962, the Accelerating Rate Calorimeter (ARC), invented by scientists from DOW Chemical in the late 1960's and the ARSST, invented by Fauske & Associates, LLC (FAI) in the early 1980's.

The Carius tube apparatus works by placing approximately 10 grams of sample in a heavy-walled, sealed glass tube and then placing it in an oven. The oven temperature is ramped at a controlled rate, typically 0.5 K/min. Temperature and pressure of the test cell are monitored and recorded in order to assess the thermal stability of a test sample upon heating. Speaking of heat – it is an interesting aside that George Ludwig Carius worked for several years with Richard Bunsen (of Bunsen burner fame).

So, getting back to the task at hand, the Carius tube method is most popular in Europe, where a preponderance of existing data from the device leads companies to perform this test on new samples in order to have a benchmark for reactivity. Like a master carpenter, a full service testing lab will have all of the tools in the shop to help customers solve process safety problems, no matter how simple or complex they may seem.

If you'd like further information regarding Carius tube testing or other services offered by FAI, please contact Dave Dale at dave@scimed.co.uk or Jeff Griffin at griffin@fauske.com. www.fauske.com.

David Dale, MSc worked for 30 years as a process safety advisor for Pfizer before joining Scientific and Medical Products (SciMed) in 2007

Jeff Griffin, MBA is Global Director of Business Development and Strategy for Fauske & Associates, LLC.

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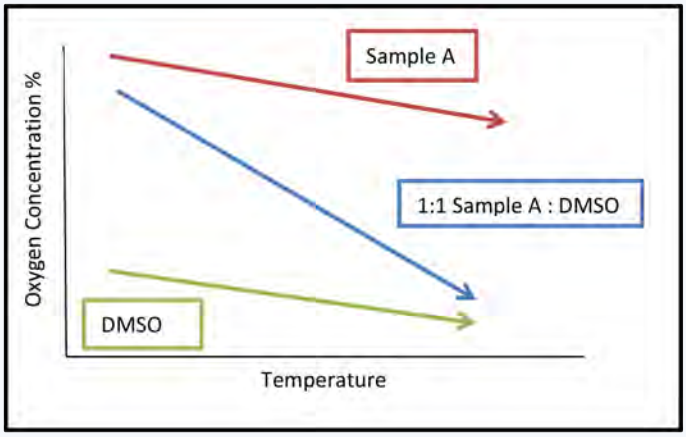
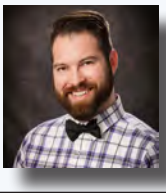
However as the temperature increases, so too does the vapor pressure of the DMSO. Thus, the partial pressure of the vapor is comprised more of DMSO molecules. The LOC of the mixture will begin to drastically decrease, moving away from the LOC of Sample A and beginning to reflect an LOC closer to that of DMSO.

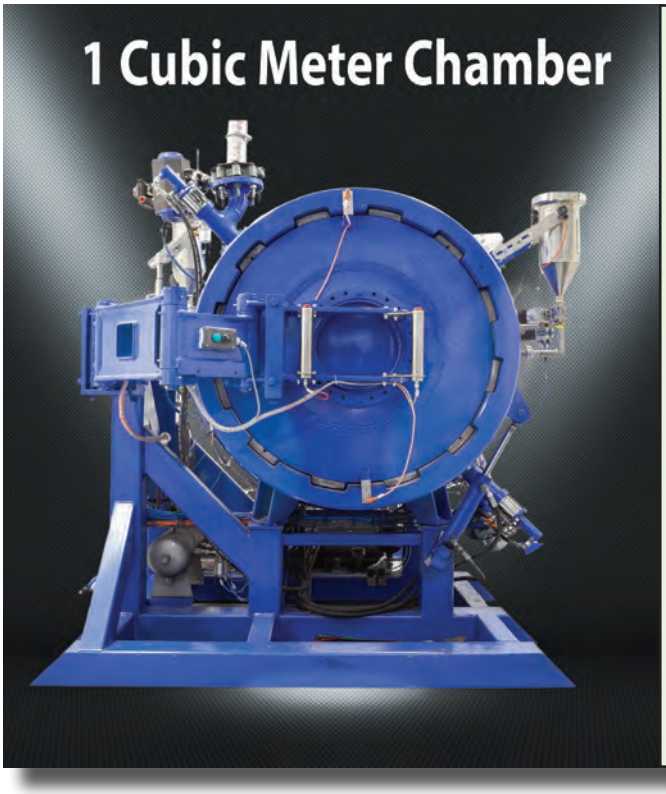
The moral of the story is to beware when working with DMSO within a process. It is a very useful and diverse product that spans industries. The presence of DMSO drastically lowers the LOC of a mixture as temperatures increase.

For more information on FAI flammability services, contact T.J. Frawley at 630-887-5289 or frawley@fauske.com.





T.J. Frawley is the Flammability Project and Lab Manager, at Fauske & Associates, LLC



FAI Product Spotlight

This is our cubic meter chamber, one of only a few in the United States. The Cubic Meter Chamber ($1m^3$) is used to verify the results found in the smaller 20-L test vessel. As a general rule, K_{St} values less than 50 would be a good candidate to verify the testing results in the cubic meter chamber. The reason for the verification is due to the small size of the 20-L chamber. It is possible to have "overdriving" or "underdriving" on your sample. Overdriving occurs when the ignition source used to conduct the experiment in the 20-L chamber preheats the material and burns the dust cloud under study without really generating a propagation flame. The second limitation, "underdriving", where the walls of the 20-L chamber abstract heat from the dust cloud explosion and partially quenches the intensity of the deflagration. The vast majority of dust and powders are not affected by these limitations. The tests performed in the cubic meter chamber include the Screening Test, also known as the Challenge Test along with K_{St}, Minimum Explosible Concentration (MEC) and Limiting Oxygen Concentration (LOC). Contact dust@fauske.com to learn more.

Fauske & Associates, LLC (FAI) Parts & Consumables Prices Set to Increase in 2018

Effective January 1, 2018, new pricing on FAI parts located in our store will be take effect. New 2018 pricing will be available by December 1, 2017.

Many of our suppliers have been passing on significant price increases due to material/labor/quality costs. We are currently conducting a detailed price analysis of our offerings.

We are doing our best to keeping pricing fair and competitive and we thank you for your understanding.

Please contact Kris Fauske at 630-887-5213 or kfauske@fauske.com with any questions.

Stock up on parts & consumables at 2017 prices through December 31, 2017

parts@fauske.com

Have You Checked Out the Fauske & Associates, LLC (FAI) Blog Lately?

We regularly publish blogs on our website addressing timely and relevant industry topics. The top five blogs visited in September ranked by page view include:

- **K_{st} and P_{max} Tests For Combustible Dust: Who or What Are They?**
- **Flammability Testing: Flash Point versus Auto-ignition Temperature**
- **FAI University Courses, Conferences & Custom Training**
- **MIT, LIT, MIE - Characterizing for Dust Hazard Analysis DHA**
- **How to Scale-up Chemical Reactions/ Runaway Reactions in a Safer Way**

Click on each title to read these posts or visit
http://www.fauske.com/blog
to read or subscribe to all of our blogs.

Fauske & Associates, LLC (FAI)is always improving our facilities. In this picture, a crane positions an upgraded Make-Up Air Unit (MAU) on the roof of our state-of-the–art flammability lab to increase the safety of the exhaust system when handling chemicals in the lab.

REACTION CALORIMETRY VS. ADIABATIC CALORIMETRY: WHICH METHOD IS RIGHT FOR ME?

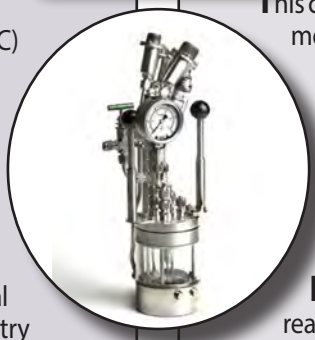
By: Donald J. Knoechel, Ph.D. , Senior Consulting Engineer &
R. Gabriel (Gabe) Wood, Manager, Thermal Hazards Testing and Consulting, Fauske & Associates, LLC

When gathering process safety information on an existing chemical process or for developing a new chemical process, the technique to choose and type of experiment to run is highly dependent on what is the intended use of the data. In this article we highlight important differences between the data from reaction calorimetry and adiabatic calorimetry and how best to use it.

The reaction calorimeters in the FAI toolbox are the Mettler-Toledo RC1, ChemiSens CPA202, and the Thermal Hazards Technology µRC. The adiabatic calorimeters are the Vent Sizing Package (VSP2), Advanced Reactive System Screening Tool (ARSST) and Accelerated Rate Calorimeter (ARC).

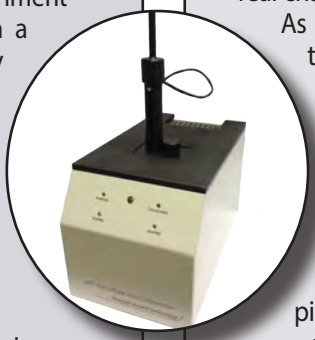
Mettler-Toledo RC1

First and foremost, **reaction calorimetry** (RC) seeks to quantify the heat evolved and the rate of heat evolution from a chemical process reaction under **desired reaction conditions**. **Adiabatic calorimetry** (AC) by definition does not hold the reaction conditions (temperature) constant and generally is used to explore the **undesired runaway scenario** (loss of cooling, overcharging, heating by external fire). The overlap between adiabatic calorimetry and reaction calorimetry lies in the fact that the adiabatic experiment often but not exclusively has the desired reaction as the trigger for runaway. In contrast, the reaction calorimetry experiment maintains temperature control to stay within a predefined temperature range where primarily only the desired chemistry takes place.



ChemiSens CPA202

The adiabatic temperature rise (ΔT_{ad}) is a deliverable from either reaction calorimetry or adiabatic calorimetry but differs in its origin and meaning depending on which technique was used.



µRC

Reaction calorimetry **measures** the **heat** evolved under a predefined set of reaction conditions (often isothermal but not necessarily) and **calculates** an **adiabatic temperature rise** from the total heat, the mass and the heat capacity (also measured in a RC experiment). The total heat can be normalized to mass or moles of limiting reagent to afford a **heat of reaction**.

Adiabatic calorimetry **measures** the **temperature rise** as a direct consequence of the experiment though the measured value is often further corrected by heat absorbed by the test cell (via the Φ - factor) to project the **true adiabatic value**. Knowing the mass and a heat capacity allows the **calculation** of the total heat that caused the temperature rise and normalizing this by mass or moles of limiting reagent yields a **heat of reaction**.

It is important to realize that the adiabatic temperature rise projection from reaction calorimetry only allows for heat from the desired reaction to contribute to the temperature rise (if any). Consequently, it does not represent the entire runaway scenario but only a minimum possible value.

This calculated temperature rise from RC differs from what is measured in adiabatic calorimetry. During the adiabatic experiment further reactions may be initiated (with their own heat of reaction) when the actual rise in temperature is experienced which may contribute to a further increase in temperature (and pressure) until all reacting/decomposing components are consumed.

Note also that the adiabatic potential projection from reaction calorimetry is based on the heat capacity at the desired reaction temperature where the adiabatic experiment experiences the temperature rise over the actual range in temperature and the corresponding real change in reaction mass heat capacity with temperature. As heat capacity generally increases with temperature, the ΔT_{ad} from RC is usually an overestimate of what the real temperature rise would be when only the desired reaction is involved.

The primary use for reaction calorimetry data is for purposes of **heat rate scale up**. That is projecting the **cooling capacity required** for running the process in larger equipment, from lab to kilolab to pilot plant to full-scale plant in order to maintain the desired temperature control.

RC also provides a unique window into the trajectory of the reaction. Issues encountered when considering RC data include the following: does the way the process is carried out (batch versus semi-batch) need to be changed with scale? Does an addition time need to be longer at larger scale? If so, is product of the same impurity profile produced with the longer addition time compared to that from the smaller scale (shorter add time).

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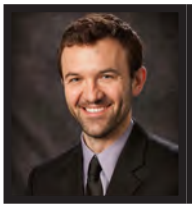

Congratulations to Damian Stefanczyk on obtaining a National Council of Examiners for Engineering and Surveying (NCEES) profile for his PE license. This allows him to easily apply for a PE license in any state and territory in the United States. Thus, if you have any project that would require a PE, we are able to accommodate those requirements upon Damian receiving approval from each state's or territory's specific board. Damian currently holds PE licenses in Illinois and Alabama.

Fauske & Associates, LLC Connected to the Community

Fauske & Associates, LLC hosted a "Back to School Supply Drive." A large number of supplies along with a monetary donation were presented to People's Resource Center in Westmont, IL (http://www.peoplesrc.org), who distributed supplies as needed to underprivileged families and /or schools in our community.

In September, Fauske & Associates, LLC employees took to the streets for the annual Willowbrook/ Burr Ridge Kiwanis Peanut Days to help support their mission to "improve the world one child and one community at a time."

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Do transient solids formation present a mixing challenge and might that change with a longer addition time? Does reversing the addition alleviate those concerns? Do any changes in heat flow (or vent flow or pH, also) correspond to points of stoichiometric equivalency?

VSP2

The projected ΔT_{ad} value from RC best serves in a screening role. A process that projects low adiabatic potential from RC may be deemed safe as long as there is complimentary thermal screening results, Differential Scanning Calorimetry (DSC), for instance, indicating minimal to no thermal activity at higher temperatures from a scan of a post-reaction mixture. On the other hand, any projected temperature rise which threatens the boiling point of the reaction mass, an understanding as to whether the reaction mass could temper the runaway would require an open adiabatic test to confirm. A potential temperature rise that could go well beyond the boiling point of the reaction mass deserves a closed adiabatic test to see how high the temperature and pressure might get and what other reactions if any might be encountered.

ARSST

Ultimately the purpose of an adiabatic test is to gather data on temperature and pressure rise (and rates thereof) for the runaway scenario. Low Φ - factor adiabatic calorimetry (ARSST, VSP2) is ideal for direct scaling up of the data. The low Φ - factor test minimizes the correction needed for heat loss to the test cell maximizing the quality of the data collected over the temperature rise by more closely simulating the thermal inertia of the large scale process vessel. Typically this type of data is desired when the process scale is known and design of the vent for a particular reactor configuration is requested. ARSST are used in a screening capacity to quickly probe different scenarios. However, ARC and ARSST are used in a screening capacity to quickly probe different scenarios. ARC is more commonly used with pure materials to probe decomposition kinetics for storage and stability concerns. ARSST is better equipped to handle mixtures and to capture data while adding reagents at the process temperature.

Fauske & Associates, LLC maintains a toolbox and the expertise to characterize your chemical processes with reaction calorimentry, adiabatic calorimetry or both as needed supported by thermal screening techniques, as well. If you have process scale up or safety concerns that suggests reaction calorimetry, please contact Don Knoechel at knoechel@fauske.com or 630-887-5251 to discuss your process. If you have vent sizing or other adiabatic testing or thermal screening needs, please contact Gabe Wood at 630-887-5270 or email at wood@fauske.com.

Don Knoechel is senior Consulting Engineer and Growth Leader for Reaction Calorimetry Testing & Consulting Services at Fauske & Associates, LLC

R. Gabriel (Gabe) Woods is Manager, Thermal Hazards Testing and Consulting at Fauske & Associates, LLC