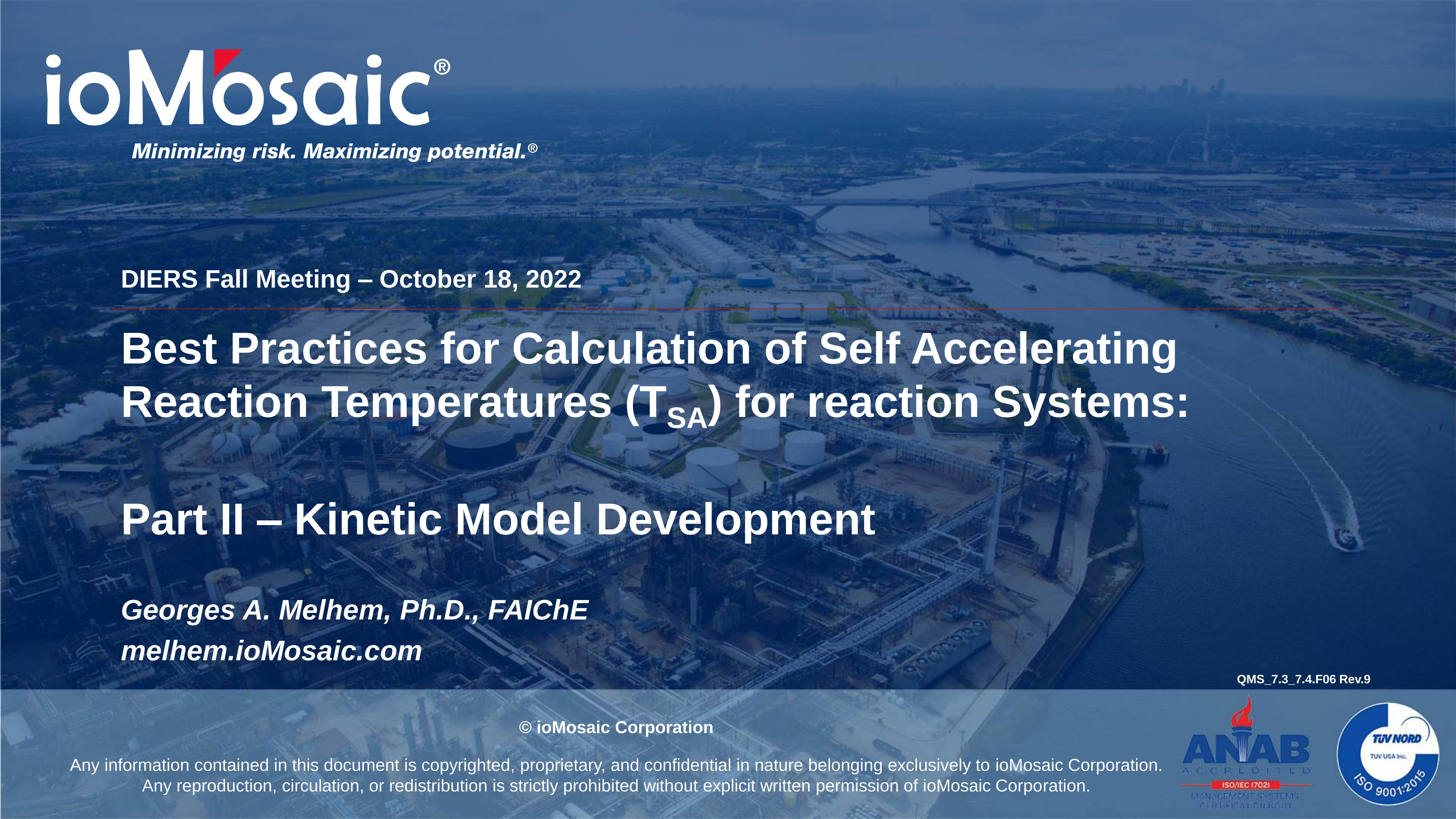

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DIERS Fall Meeting – October 18, 2022

Best Practices for Calculation of Self Accelerating Reaction Temperatures (T_{SA}) for reaction Systems:

Part II – Kinetic Model Development

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- PRV Stability and Fluid Dynamics
- Chemical Reaction Systems
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G. A. Melhem, Ph.D., FAIChE
President and CEO

This tutorial represents part I of a six-part series on “Best Practices for Calculation of Self Accelerating Reaction Temperatures (T_{SA}) for Reaction Systems”

- Part I – Data Reduction
- Part II – Kinetic Model Development
- Part III – Semenov Approach, Simplified and Dynamic
- Part IV - Kamenetskii Approach, 1D/2D, Simplified and Dynamic
- Part V – Case Studies
- Part VI – UN and DOT Requirements

What you are expected to learn from this tutorial includes

- How to develop simple iso-conversion kinetic models
- How to develop thermal stability indicators including T_{SA}, T_{NR}, and t_{MR}
- How to evaluate thermal stability
- How to develop detailed kinetic models
- How to use detailed kinetic models for pressure relief systems design and evaluation

Key References:

G. A. Melhem, S. Grenier, and L. Ding, *"Thermal stability indicators",* an ioMosaic Corporation white paper, August 2021.

G. A. Melhem, "*Development of kinetic models – Part I. Thermal Stability*", an ioMosaic Corporation white paper, August 2022.

G. A. Melhem, "*Development of kinetic models – Part II. Pressure Relief Systems*", an ioMosaic Corporation white paper, August 2022.

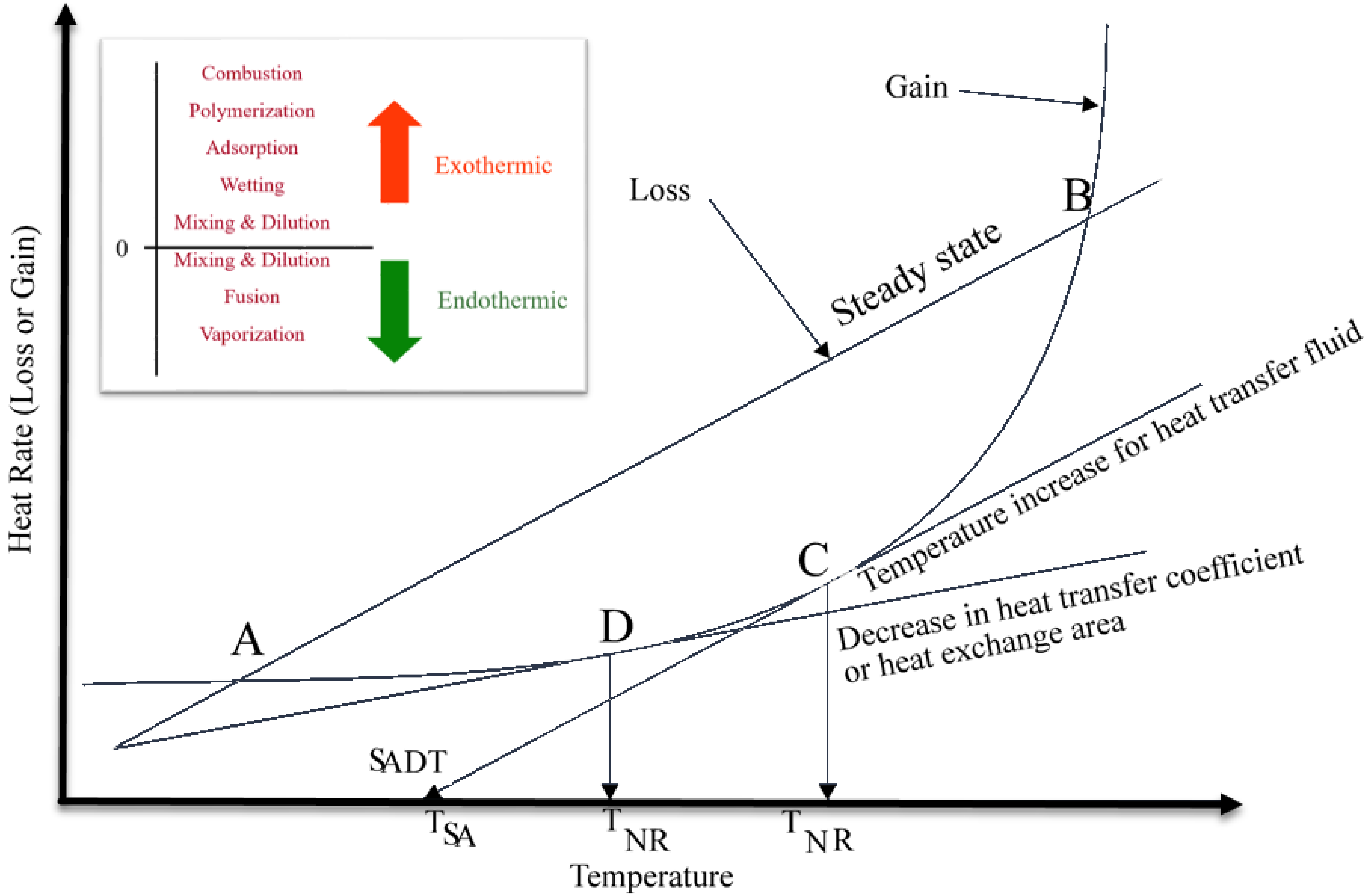
Why do we need kinetic models?

- Exothermic runaway reactions can cause loss of containment, significant loss of property and life, and environmental impact
- Safe storage, handling, and transportation of reactive chemicals require rate information for both desired and undesired chemistries
- Safe Scaleup of laboratory data to plant scale
- Numerous scenarios can cause runaway reactions
- Safe discharge location considerations

What kind or types of kinetic models can be developed from calorimetry data?

Reaction rates are significantly influenced by temperature

- Simple or isoconversion models
- Detailed models
- ~~Mechanistic?~~



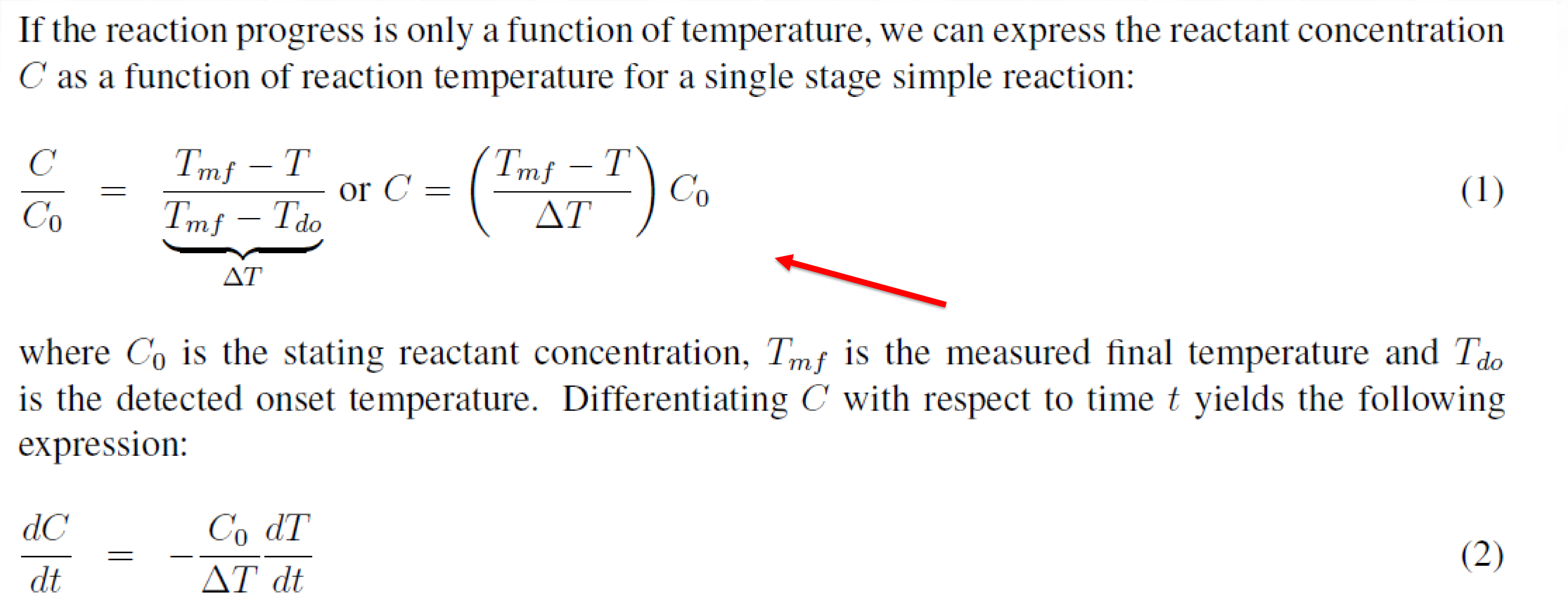
Simple or isoconversion models are easy to develop but …

- Cannot be used for pressure relief design and/or vent containment design
- Mostly used for thermal stability assessments where phase change can be neglected and where there is no mass exchange with the system boundaries
- Do not require information about stoichiometry, phase change, or vapor/liquid equilibrium
- Requires calorimetry data (ISO Laboratories recommended) as do detailed models

Detailed kinetic models are more complex than isoconversion models, but..

- They can be used to extend limited test data to wider ranges of composition, temperature, and pressure
- Require the development of reaction stoichiometry, and detailed thermophysical and transport properties
- Mostly used for modeling the dynamics of pressure relief systems and/or vent containment design, process dynamics, as well as thermal stability assessments
- Recommended over direct scale-up models because they often result in practical designs and better risk reduction
- Once a detailed kinetic model is developed, it can be used repeatedly in many process design and modeling applications

Temperature based isoconversion models assume that conversion of reactants is only a function of temperature



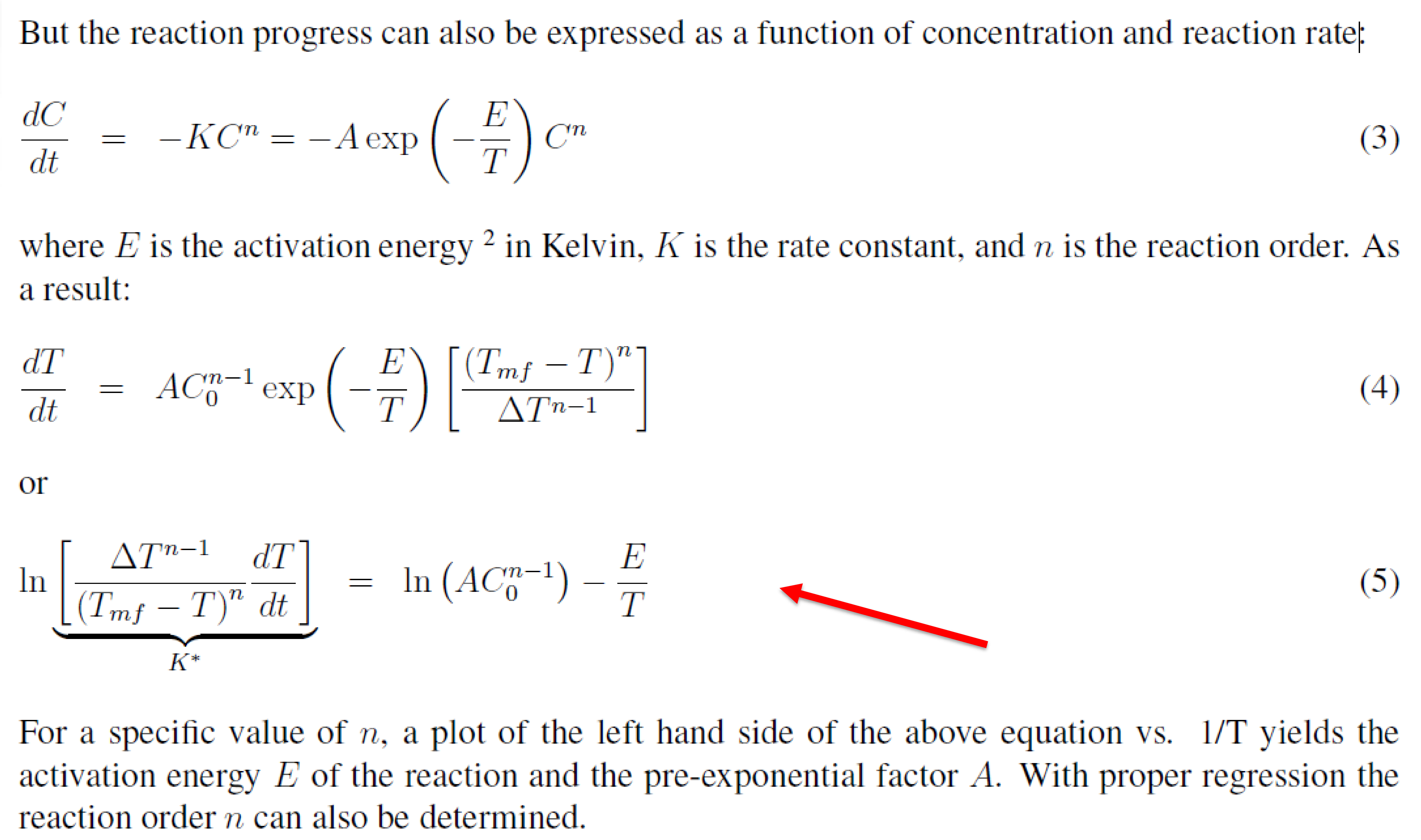
If the reaction progress is only a function of temperature, we can express the reactant concentration C as a function of reaction temperature for a single stage simple reaction:

$$\frac{C}{C_0} = \frac{T_{mf} - T}{\underbrace{T_{mf} - T_{do}}_{\Delta T}} \text{ or } C = \left(\frac{T_{mf} - T}{\Delta T}\right) C_0 \tag{1}$$

where C_0 is the stating reactant concentration, T_{mf} is the measured final temperature and T_{do} is the detected onset temperature. Differentiating C with respect to time t yields the following expression:

$$\frac{dC}{dt} = -\frac{C_0}{\Delta T}\frac{dT}{dt} \tag{2}$$

But the reaction progress can also be expressed as a function of concentration and reaction rate



But the reaction progress can also be expressed as a function of concentration and reaction rate:

$$\frac{dC}{dt} = -KC^n = -A\exp\left(-\frac{E}{T}\right)C^n \qquad (3)$$

where E is the activation energy [2] in Kelvin, K is the rate constant, and n is the reaction order. As a result:

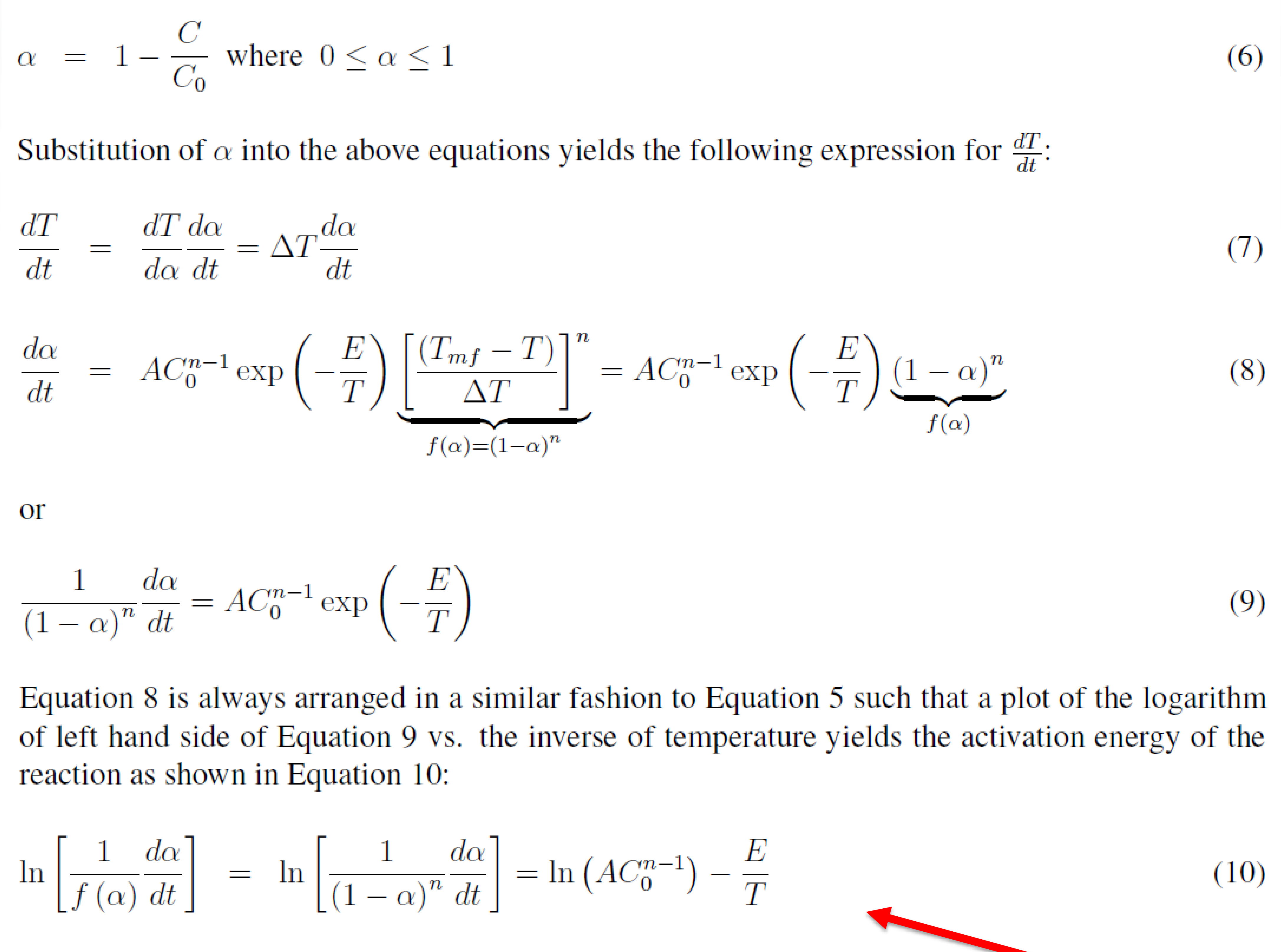
$$\frac{dT}{dt} = AC_0^{n-1}\exp\left(-\frac{E}{T}\right)\left[\frac{(T_{mf}-T)^n}{\Delta T^{n-1}}\right] \qquad (4)$$

or

$$\underbrace{\ln\left[\frac{\Delta T^{n-1}}{(T_{mf}-T)^n}\frac{dT}{dt}\right]}_{K^*} = \ln\left(AC_0^{n-1}\right) - \frac{E}{T} \qquad (5)$$

For a specific value of n, a plot of the left hand side of the above equation vs. 1/T yields the activation energy E of the reaction and the pre-exponential factor A. With proper regression the reaction order n can also be determined.

Isoconversion models relate the reaction progress or conversion to concentration



$$\alpha \;=\; 1-\frac{C}{C_0} \quad \text{where} \;\; 0 \leq \alpha \leq 1 \tag{6}$$

Substitution of α into the above equations yields the following expression for $\frac{dT}{dt}$:

$$\frac{dT}{dt} \;=\; \frac{dT}{d\alpha}\frac{d\alpha}{dt} = \Delta T \frac{d\alpha}{dt} \tag{7}$$

$$\frac{d\alpha}{dt} \;=\; AC_0^{n-1}\exp\left(-\frac{E}{T}\right)\underbrace{\left[\frac{(T_{mf}-T)}{\Delta T}\right]^n}_{f(\alpha)=(1-\alpha)^n} = AC_0^{n-1}\exp\left(-\frac{E}{T}\right)\underbrace{(1-\alpha)^n}_{f(\alpha)} \tag{8}$$

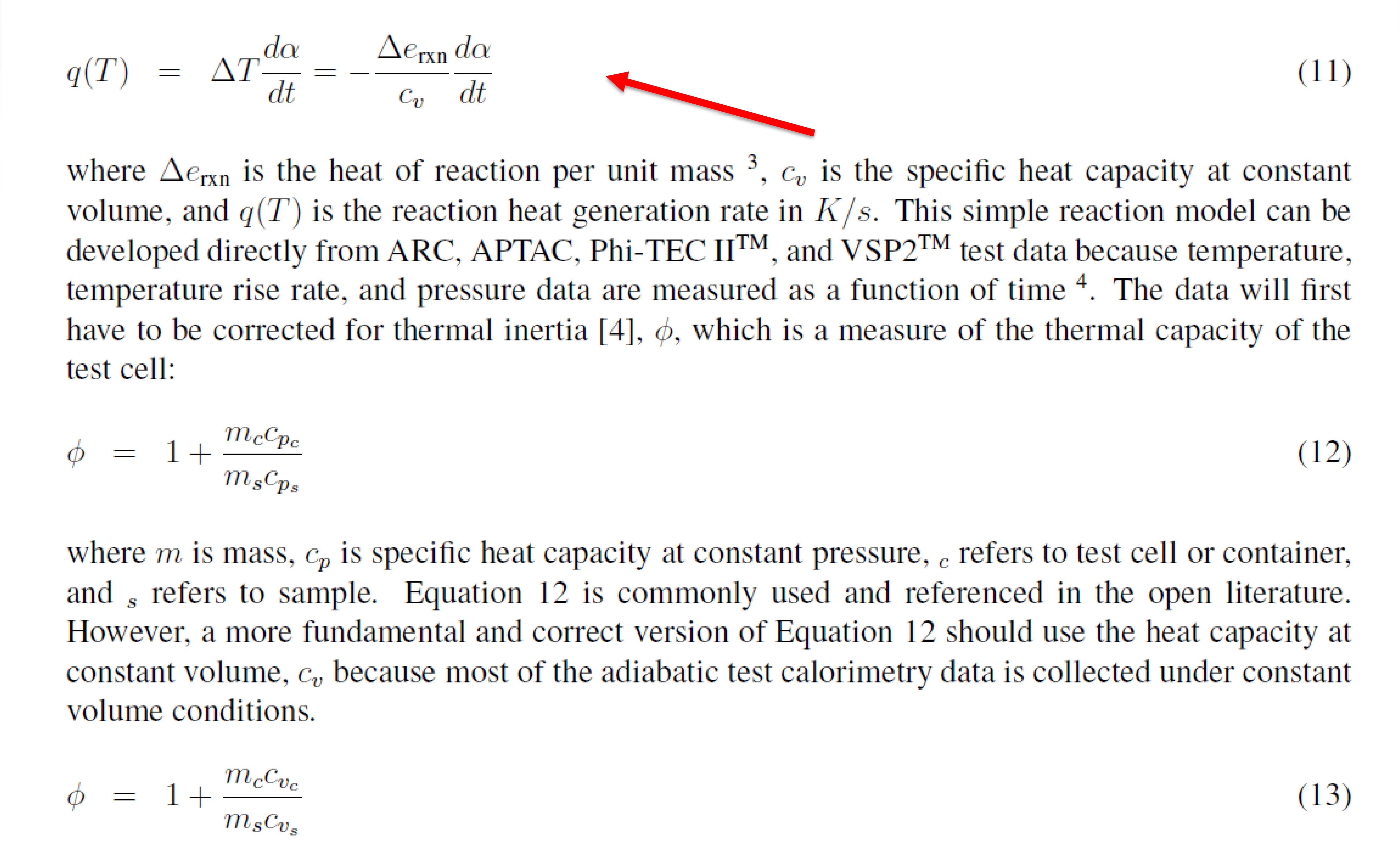
or

$$\frac{1}{(1-\alpha)^n}\frac{d\alpha}{dt} = AC_0^{n-1}\exp\left(-\frac{E}{T}\right) \tag{9}$$

Equation 8 is always arranged in a similar fashion to Equation 5 such that a plot of the logarithm of left hand side of Equation 9 vs. the inverse of temperature yields the activation energy of the reaction as shown in Equation 10:

$$\ln\left[\frac{1}{f(\alpha)}\frac{d\alpha}{dt}\right] \;=\; \ln\left[\frac{1}{(1-\alpha)^n}\frac{d\alpha}{dt}\right] = \ln\left(AC_0^{n-1}\right) - \frac{E}{T} \tag{10}$$

The reaction heating rate is expressed as a function of the overall heat of reaction and dα/dt



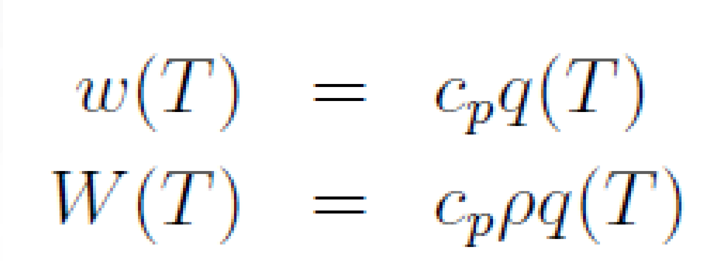
$$q(T) = \Delta T \frac{d\alpha}{dt} = -\frac{\Delta e_{\mathrm{rxn}}}{c_v}\frac{d\alpha}{dt} \tag{11}$$

where Δe_{rxn} is the heat of reaction per unit mass [3], c_v is the specific heat capacity at constant volume, and $q(T)$ is the reaction heat generation rate in K/s. This simple reaction model can be developed directly from ARC, APTAC, Phi-TEC II$^{\mathrm{TM}}$, and VSP2$^{\mathrm{TM}}$ test data because temperature, temperature rise rate, and pressure data are measured as a function of time [4]. The data will first have to be corrected for thermal inertia [4], ϕ, which is a measure of the thermal capacity of the test cell:

$$\phi = 1 + \frac{m_c c_{p_c}}{m_s c_{p_s}} \tag{12}$$

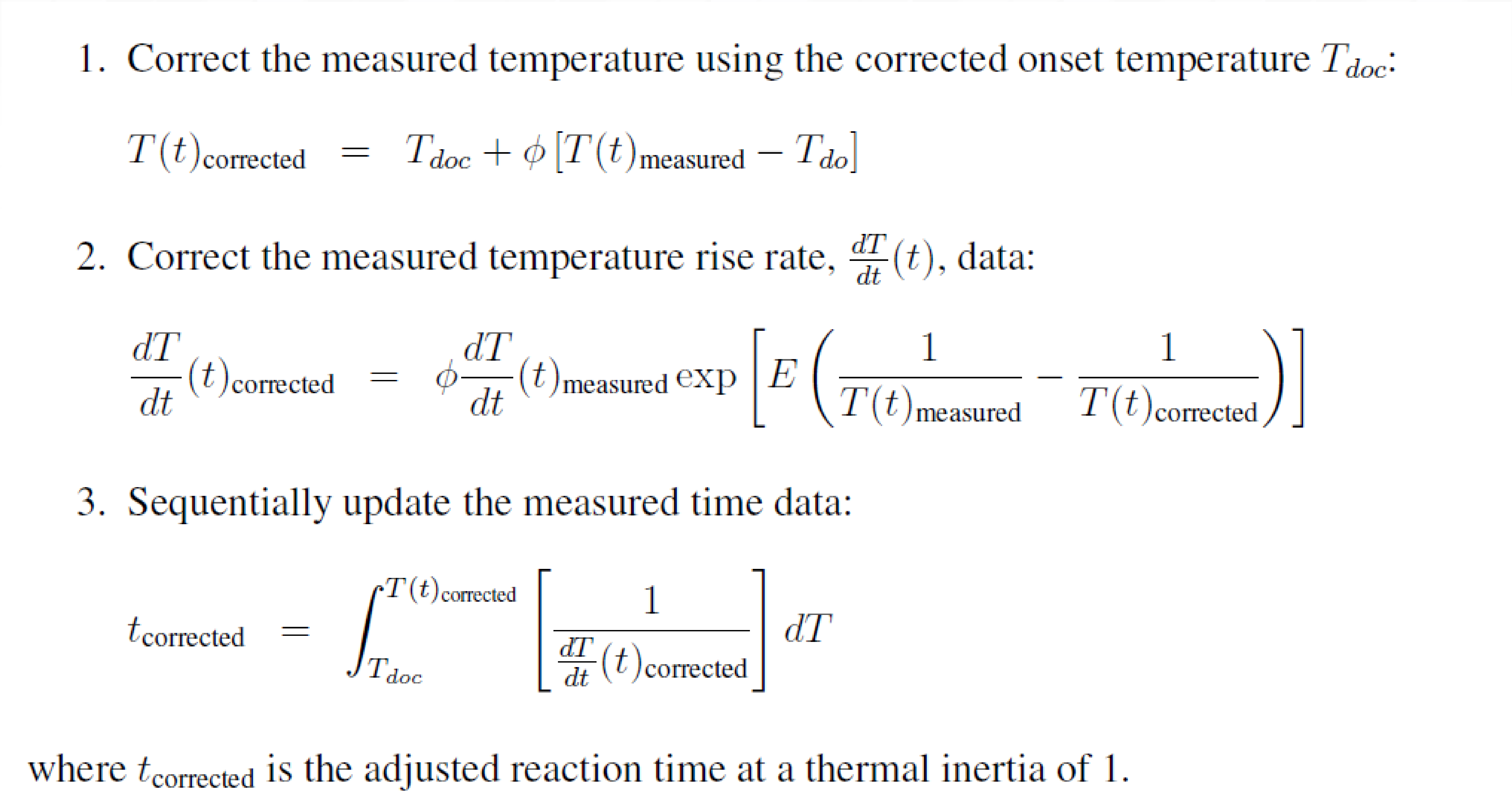
where m is mass, c_p is specific heat capacity at constant pressure, $_c$ refers to test cell or container, and $_s$ refers to sample. Equation 12 is commonly used and referenced in the open literature. However, a more fundamental and correct version of Equation 12 should use the heat capacity at constant volume, c_v because most of the adiabatic test calorimetry data is collected under constant volume conditions.

$$\phi = 1 + \frac{m_c c_{v_c}}{m_s c_{v_s}} \tag{13}$$



$$\begin{aligned} w(T) &= c_p q(T) \\ W(T) &= c_p \rho q(T) \end{aligned}$$

Measured data can also be corrected for thermal inertia for simple single stage reactions



1. Correct the measured temperature using the corrected onset temperature T_{doc}:

$$T(t)_{\text{corrected}} = T_{doc} + \phi\left[T(t)_{\text{measured}} - T_{do}\right]$$

2. Correct the measured temperature rise rate, $\frac{dT}{dt}(t)$, data:

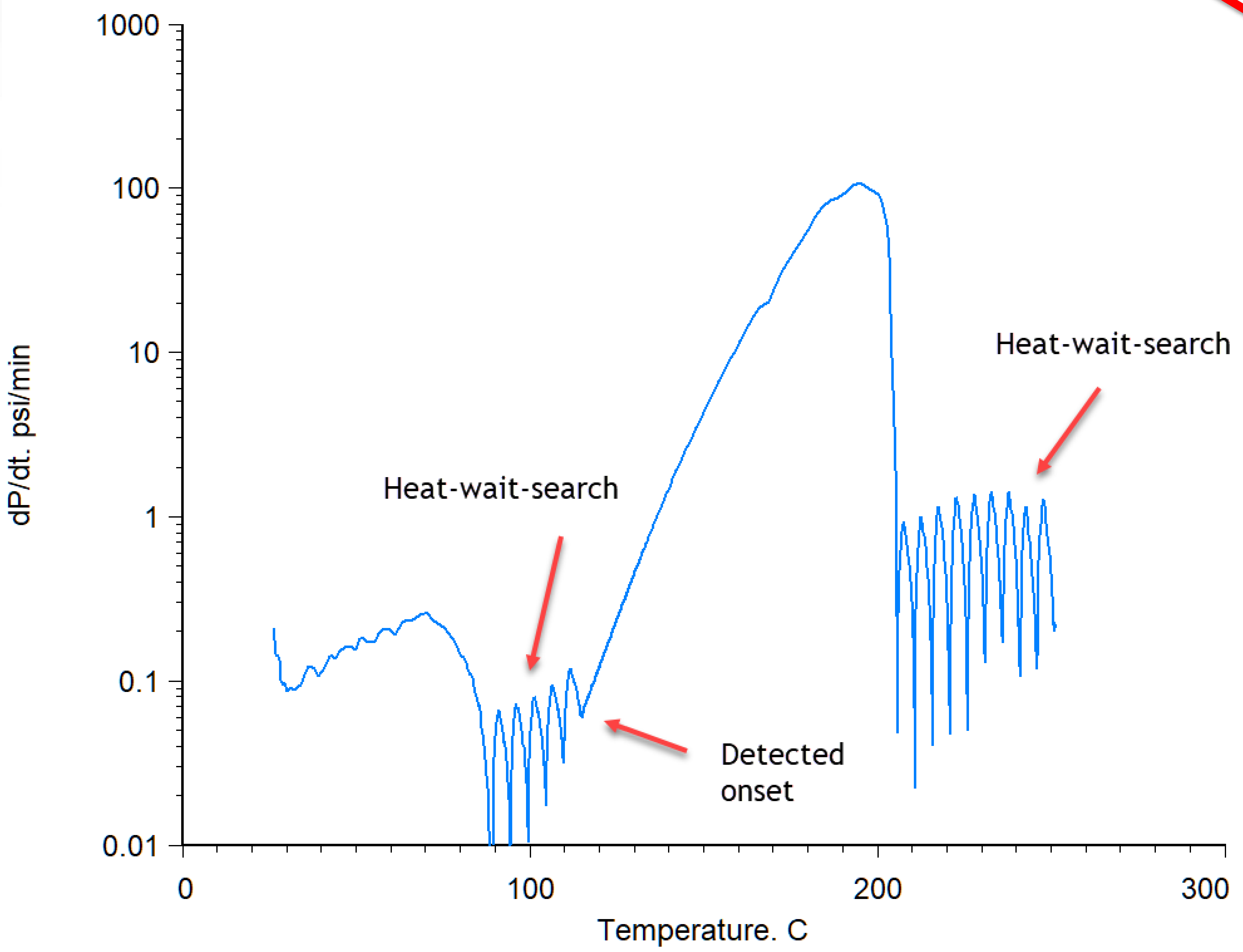
$$\frac{dT}{dt}(t)_{\text{corrected}} = \phi\frac{dT}{dt}(t)_{\text{measured}} \exp\left[E\left(\frac{1}{T(t)_{\text{measured}}} - \frac{1}{T(t)_{\text{corrected}}}\right)\right]$$

3. Sequentially update the measured time data:

$$t_{\text{corrected}} = \int_{T_{doc}}^{T(t)_{\text{corrected}}} \left[\frac{1}{\frac{dT}{dt}(t)_{\text{corrected}}}\right] dT$$

where $t_{\text{corrected}}$ is the adjusted reaction time at a thermal inertia of 1.

ARC Measured dT/dt for a 20 % mixture of di-t-butyl peroxide in toluene (φ=1.78)

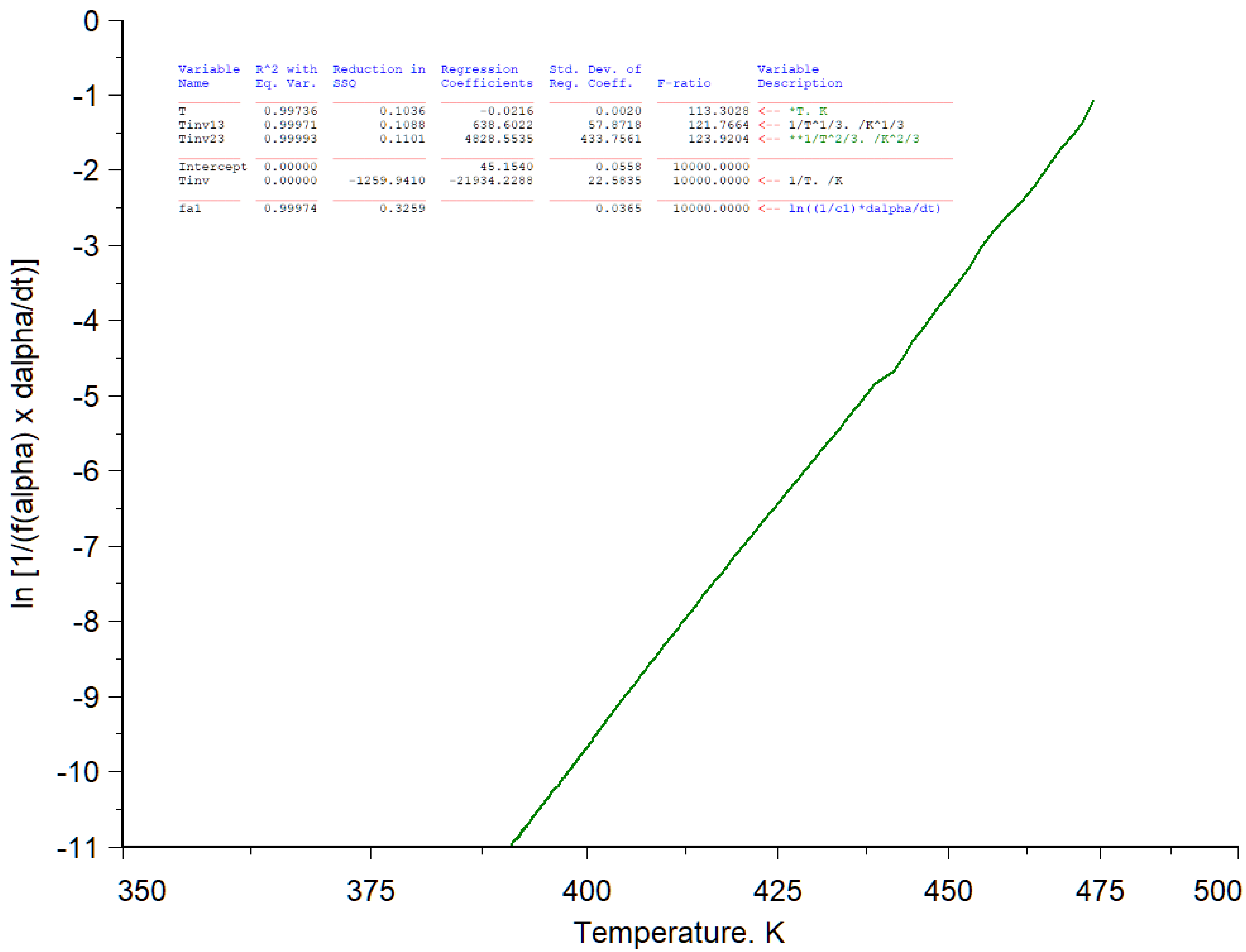


$$\frac{1}{(1-\alpha)^1}\frac{d\alpha}{dt} = \underbrace{4.075\times 10^{19}}_{A\times C_0^0}\times \exp\left(-\frac{21,934}{T}\right)$$

The first order isoconversion model parameters are shown above. The overall heat of decomposition is determined to be -1,416 J/g of di-t-butyl peroxide.

We note that the initial concentration C_0 is raised to the power n − 1 = 0 and does not influence the pre-exponential factor A

ARC data isoconversion best fit model for a 20 % mixture of di-t-butyl peroxide in toluene (φ=1.78) using SuperChems Expert



```
Variable   R^2 with  Reduction in  Regression    Std. Dev. of              Variable
Name       Eq. Var.  SSQ           Coefficients  Reg. Coeff.   F-ratio     Description

T          0.99736        0.1036       -0.0216        0.0020    113.3028  <-- *T. K
Tinv13     0.99971        0.1088      638.6022       57.8718    121.7664  <-- 1/T^1/3. /K^1/3
Tinv23     0.99993        0.1101     4828.5535      433.7561    123.9204  <-- **1/T^2/3. /K^2/3

Intercept  0.00000                     45.1540        0.0558  10000.0000
Tinv       0.00000    -1259.9410   -21934.2288       22.5835  10000.0000  <-- 1/T. /K

fal        0.99974        0.3259                      0.0365  10000.0000  <-- ln((1/cl)*dalpha/dt)
```

DSC data can also be used to develop isoconversion kinetic models based on heat flow data

$$\alpha = \frac{Q}{-\Delta e_{rxn}} \text{ or} \tag{15}$$

$$\frac{d\alpha}{dt} = \frac{\dot{Q}}{-\Delta e_{rxn}} \tag{16}$$

and

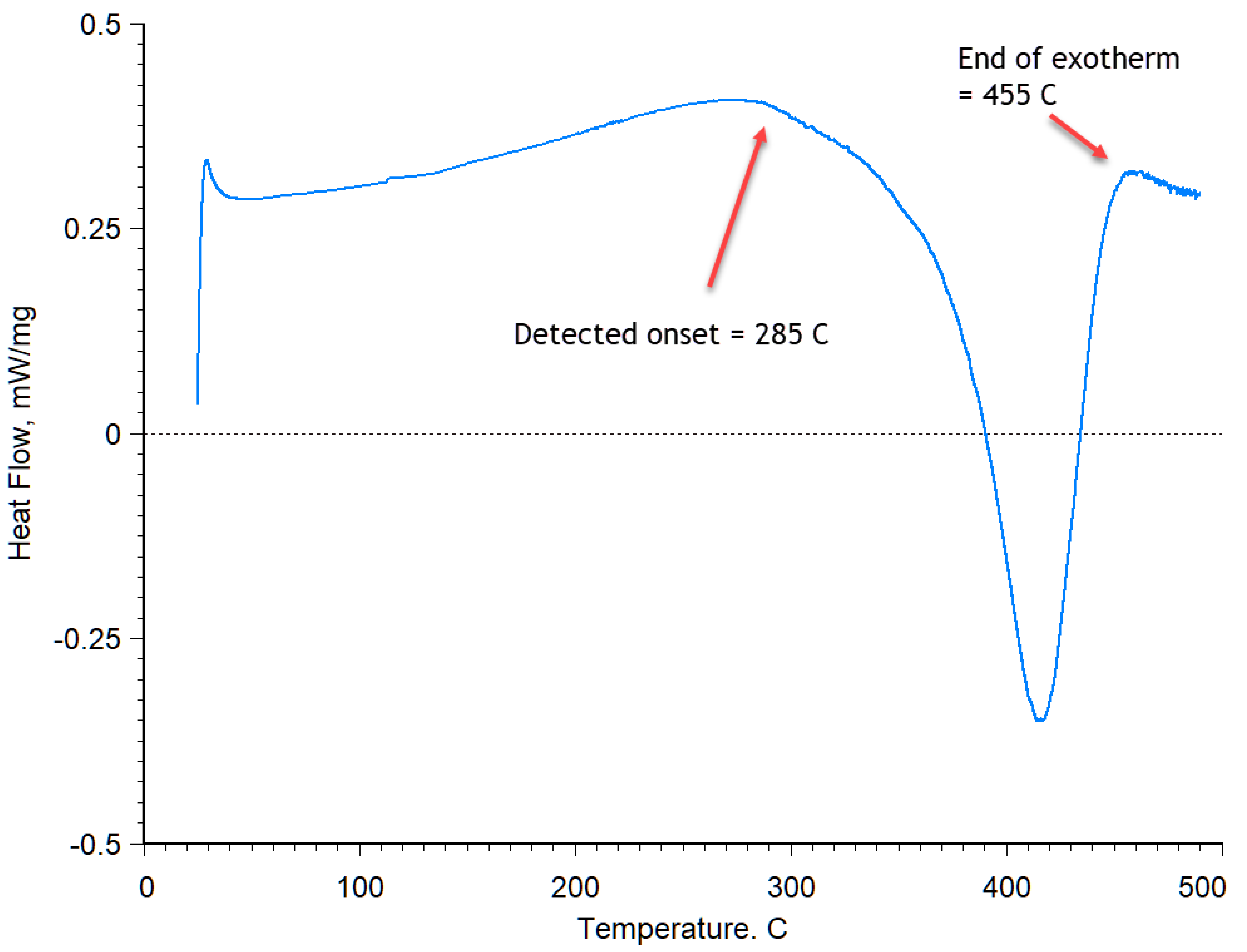
$$\ln\left(\frac{1}{f(\alpha)}\frac{d\alpha}{dt}\right) = \ln\left[A(\alpha)\right] - \frac{E(\alpha)}{T(t)} \tag{17}$$

$$T(t) = T_0 + \beta t \tag{18}$$

Integration of the conversion rate, dα/dt, yields the reaction time

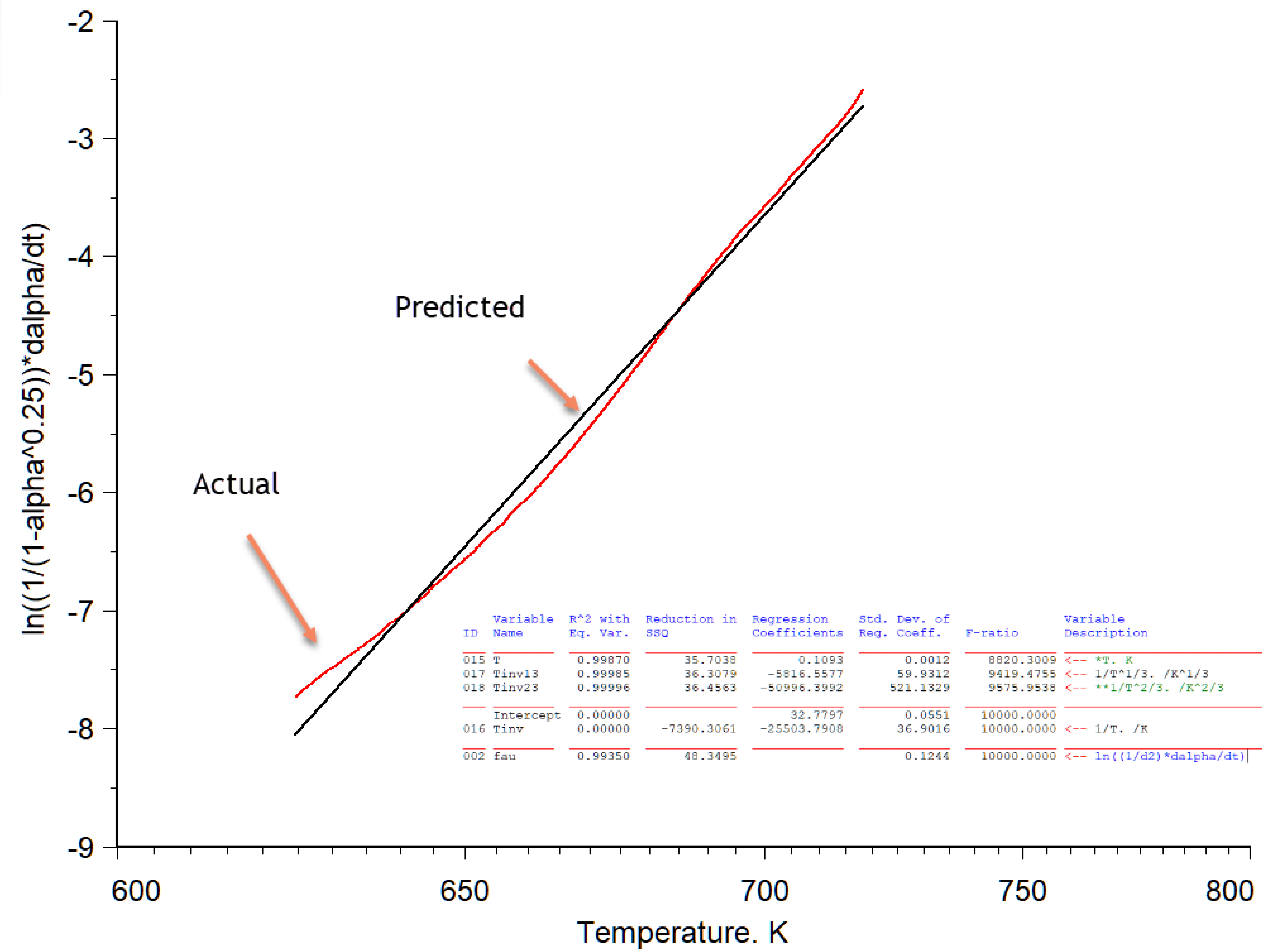
$$t = \int_0^t dt = \int_0^\alpha \left(\frac{1}{\frac{d\alpha}{dt}}\right) d\alpha = \int_0^\alpha \frac{d\alpha}{f(\alpha)A(\alpha)\exp\left(-\frac{E(\alpha)}{T(t)}\right)} \tag{19}$$

Measured DSC heat flow data for alpha-methylstyrene at a heating rate, β = 5 C/min



The integrated overall heat of reaction is approximately -430 J/g

Best fit DSC isoconversion model parameters for alpha-methylstyrene polymerization using SuperChems Expert



```
    Variable  R^2 with  Reduction in  Regression   Std. Dev. of             Variable
ID  Name      Eq. Var.  SSQ           Coefficients Reg. Coeff.   F-ratio    Description

015 T          0.99870       35.7038        0.1093       0.0012  8820.3009 <-- *T. K
017 Tinv13     0.99985       36.3079    -5816.5577      59.9312  9419.4755 <-- 1/T^1/3. /K^1/3
018 Tinv23     0.99996       36.4563   -50996.3992     521.1329  9575.9538 <-- **1/T^2/3. /K^2/3

    Intercept  0.00000                     32.7797       0.0551 10000.0000
016 Tinv       0.00000    -7390.3061   -25503.7908      36.9016 10000.0000 <-- 1/T. /K

002 fau        0.99350       48.3495                     0.1244 10000.0000 <-- ln((1/d2)*dalpha/dt)|
```

The best fit isoconversion model parameters are shown below

$$\frac{1}{\left(1-\alpha^{1/4}\right)^{1}}\frac{d\alpha}{dt} = 1.722\times10^{14}\times\exp\left(-\frac{25,504}{T}\right)$$

Similarly, mass loss data (TGA) can be used to develop simple isoconversion kinetic rate expressions

$$\begin{aligned} \alpha(T) &= \frac{m_0 - m(T)}{m_0 - m_f} \\ T(t) &= T_0 + \beta t \end{aligned}$$

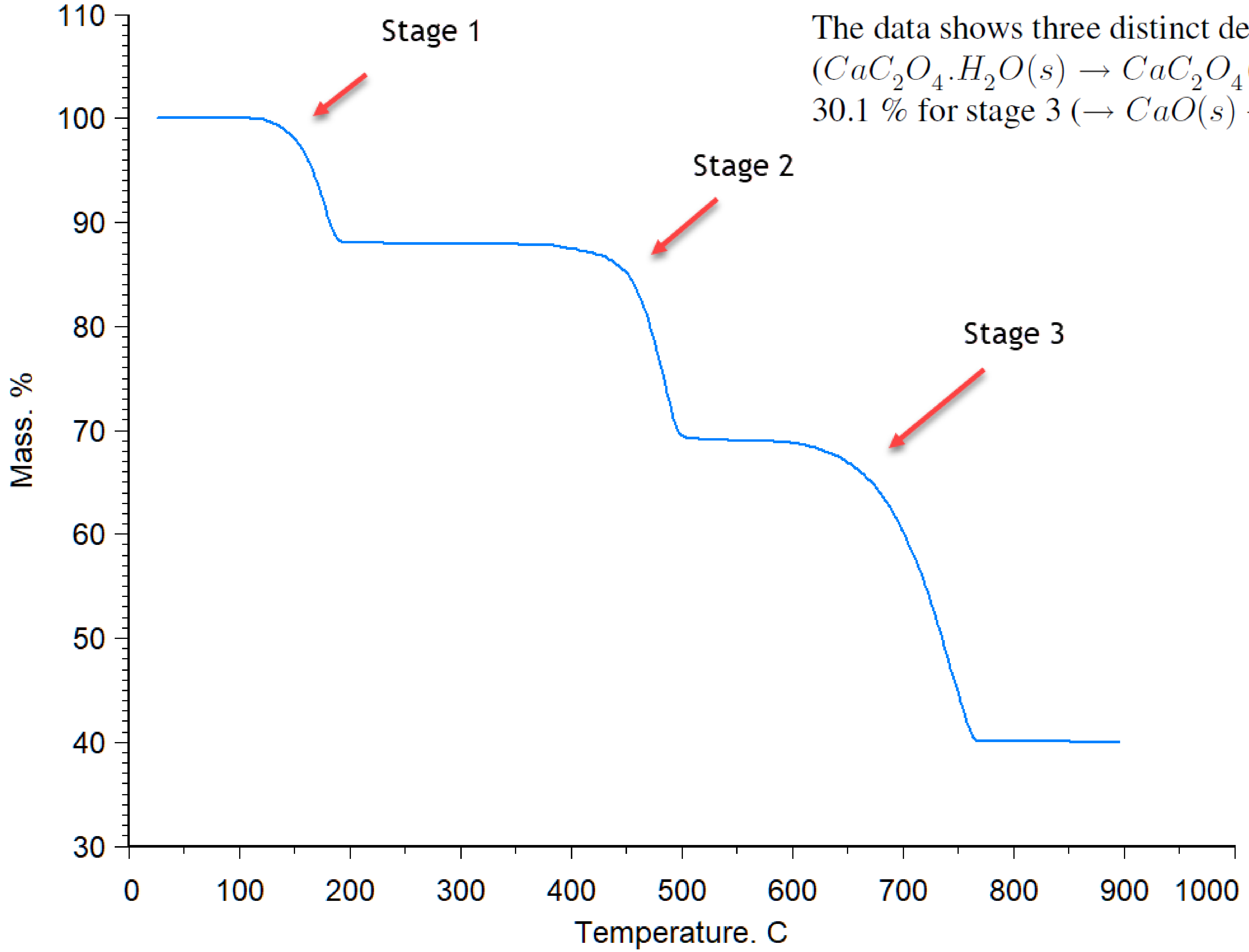
$$\frac{d\alpha}{dt} = \frac{dT}{dt}\frac{d\alpha}{dT} = \beta\frac{d\alpha}{dT}$$

$$\begin{aligned} \left(\frac{d\alpha}{dT}\right)_0 &= \frac{\alpha_1 - \alpha_0}{T_1 - T_0} \\ \left(\frac{d\alpha}{dT}\right)_i &= \frac{1}{2}\left(\frac{\alpha_i - \alpha_{i-1}}{T_i - T_{i-1}}\right) + \frac{1}{2}\left(\frac{\alpha_{i+1} - \alpha_i}{T_{i+1} - T_i}\right) \quad \text{for } i = 1, ..., n-2 \\ \left(\frac{d\alpha}{dT}\right)_{n-1} &= \frac{\alpha_{n-1} - \alpha_{n-2}}{T_{n-1} - T_{n-2}} \end{aligned}$$

Like DSC data, integration of the TGA conversion rate yields the reaction time (also see [6]):

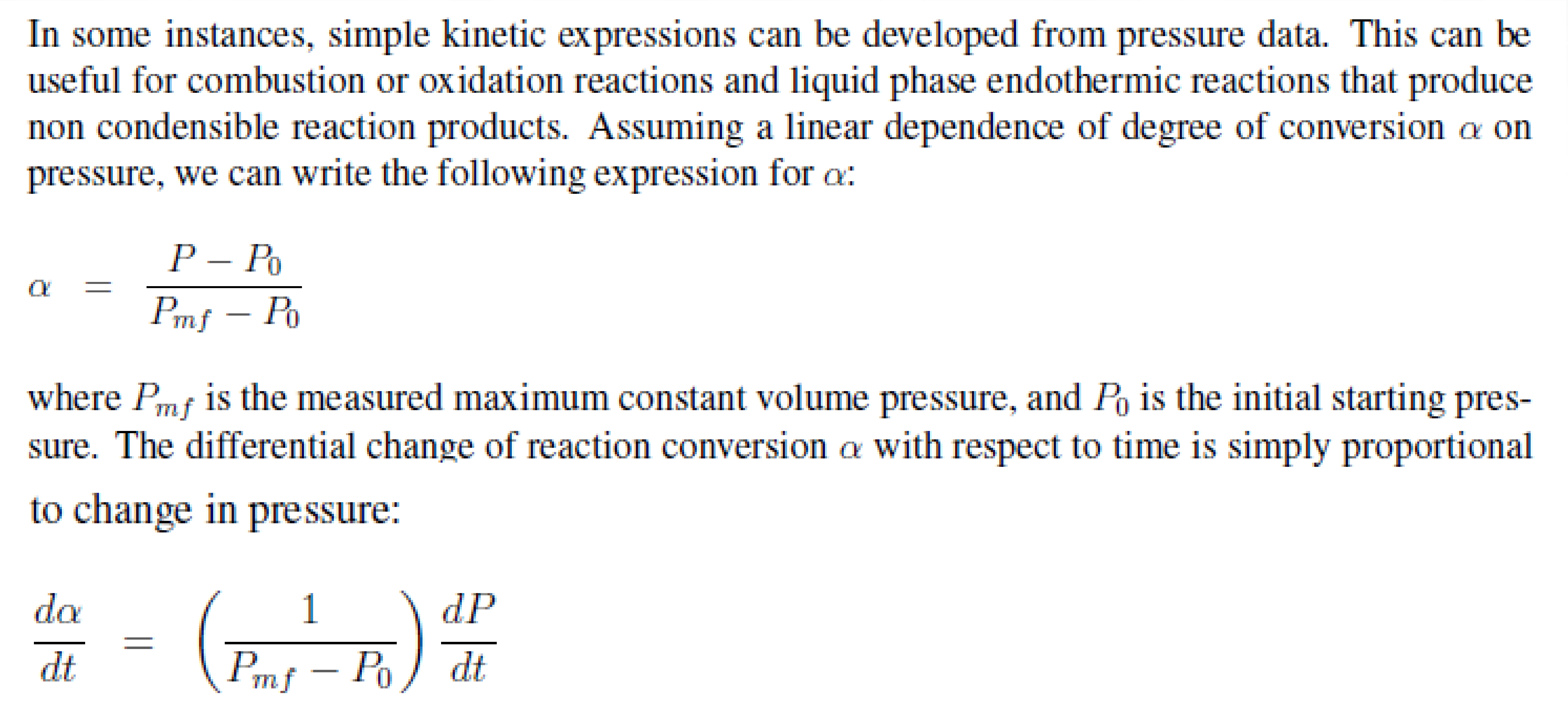
$$t = \int_0^t dt = \int_0^\alpha \left(\frac{1}{\beta\frac{d\alpha}{dT}}\right) d\alpha = \int_0^\alpha \frac{d\alpha}{A(\alpha)\exp\left(-\frac{E(\alpha)}{T(t)}\right) f(\alpha)}$$

Measured TGA mass loss data for calcium oxalate



The data shows three distinct decomposition stages of approximately 12 % weight loss for stage 1 ($CaC_2O_4.H_2O(s) \rightarrow CaC_2O_4(s) + H_2O(g)$), 19.2 % for stage 2 ($\rightarrow CaCO_3(s) + CO(g)$) and 30.1 % for stage 3 ($\rightarrow CaO(s) + CO_2(g)$).

Isoconversion kinetic models can also be developed based on measured pressure and/or pressure rates



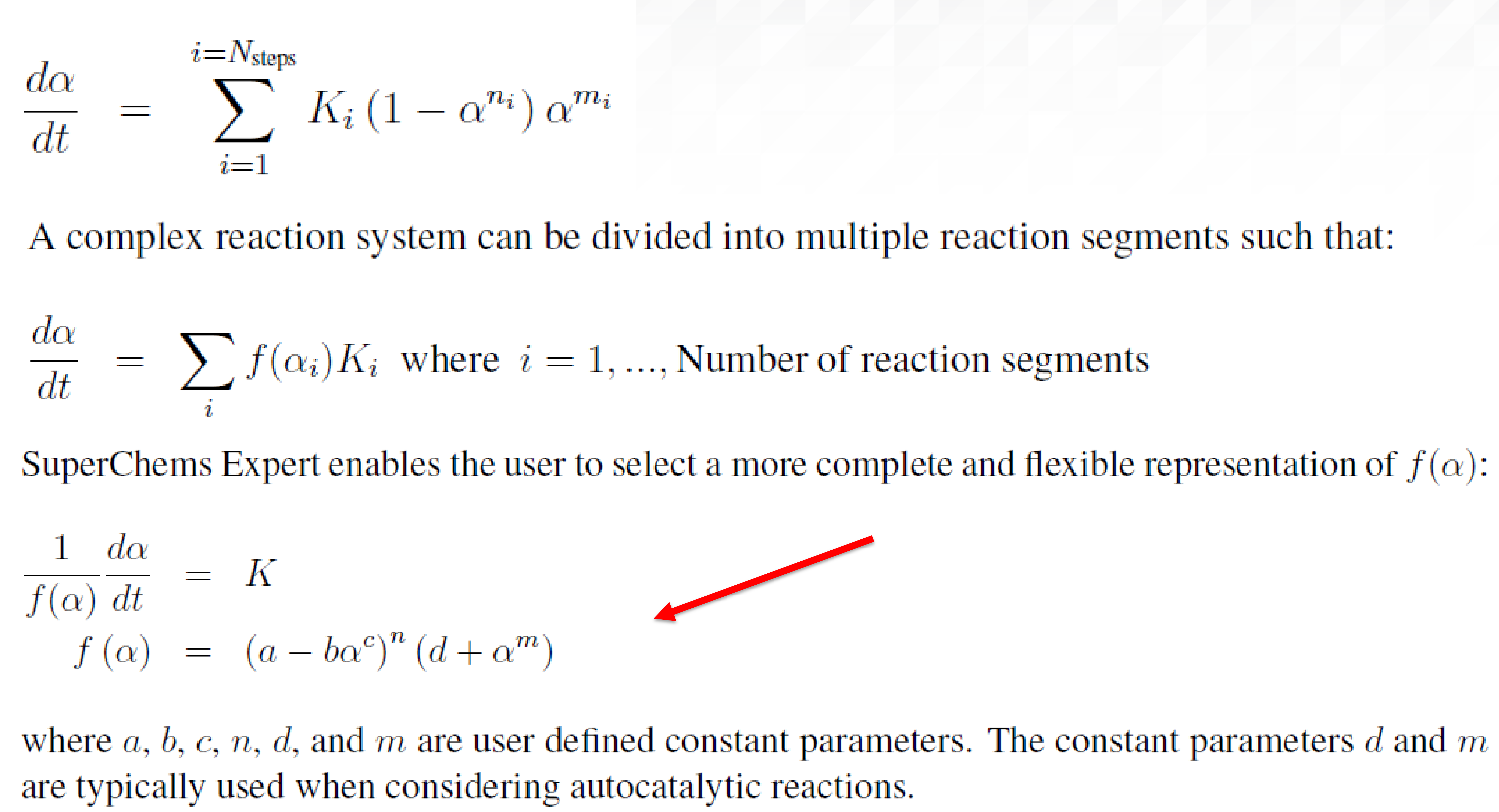
In some instances, simple kinetic expressions can be developed from pressure data. This can be useful for combustion or oxidation reactions and liquid phase endothermic reactions that produce non condensible reaction products. Assuming a linear dependence of degree of conversion α on pressure, we can write the following expression for α:

$$\alpha = \frac{P - P_0}{P_{mf} - P_0}$$

where P_{mf} is the measured maximum constant volume pressure, and P_0 is the initial starting pressure. The differential change of reaction conversion α with respect to time is simply proportional to change in pressure:

$$\frac{d\alpha}{dt} = \left(\frac{1}{P_{mf} - P_0}\right)\frac{dP}{dt}$$

More complex isoconversion forms can be used to represent multi-step reactions and reactions with autocatalytic behavior



$$\frac{d\alpha}{dt} = \sum_{i=1}^{i=N_{\text{steps}}} K_i \left(1 - \alpha^{n_i}\right) \alpha^{m_i}$$

A complex reaction system can be divided into multiple reaction segments such that:

$$\frac{d\alpha}{dt} = \sum_i f(\alpha_i) K_i \text{ where } i = 1, \ldots, \text{Number of reaction segments}$$

SuperChems Expert enables the user to select a more complete and flexible representation of $f(\alpha)$:

$$\frac{1}{f(\alpha)} \frac{d\alpha}{dt} = K$$

$$f(\alpha) = \left(a - b\alpha^c\right)^n \left(d + \alpha^m\right)$$

where a, b, c, n, d, and m are user defined constant parameters. The constant parameters d and m are typically used when considering autocatalytic reactions.

We can easily couple isoconversion models with thermal explosion theory

$$\underbrace{m_T c_{v_T}\frac{dT}{dt} + m_c c_{v_c}\frac{dT_c}{dt}}_{\text{Heat Accumulation}} = \underbrace{US\left(T_a - T_c\right)}_{\text{Heat Transfer}} - \underbrace{\frac{dm_p}{dt}\Delta e_{\text{rxn}}}_{\text{Heat Generation}}$$

$$\begin{aligned}
\frac{d\alpha}{dt} &= A(\alpha)f(\alpha)\exp\left(-\frac{E(\alpha)}{T}\right) \\
q(T) &= -\frac{\Delta e_{\text{rxn}}}{c_{v_T}}\frac{d\alpha}{dt} \quad \text{and} \\
\tau(T) &= \frac{m_T c_{v_T}}{US} \quad \text{and} \\
\frac{dT}{dt} &= \frac{1}{\phi}\left[\frac{1}{\tau(T)}\left(T_a - T\right) + q(T)\right]
\end{aligned}$$

T_{SA} is the lowest ambient or heat transfer fluid temperature above which equilibrium is lost

$$T_{SA} = T_{NR} - \frac{1}{\frac{E}{T_{NR}^2} - \frac{n}{T_f - T_{NR}} + \frac{d\ln[\tau(T_v)]}{dT_v}}\Big|_{@T_v=T_{NR}}$$

Semenov:

$$T^2 = t_{MR}(T) \times E \times q(T) \text{ or } t_{MR}(T) = \frac{T^2}{E}\frac{1}{q(T)}$$

$$T_{NR}^2 = \tau(T_{NR}) \times E \times q(T_{NR})$$

$$T_{SA} = T_{NR} - \frac{T_{NR}^2}{E}$$

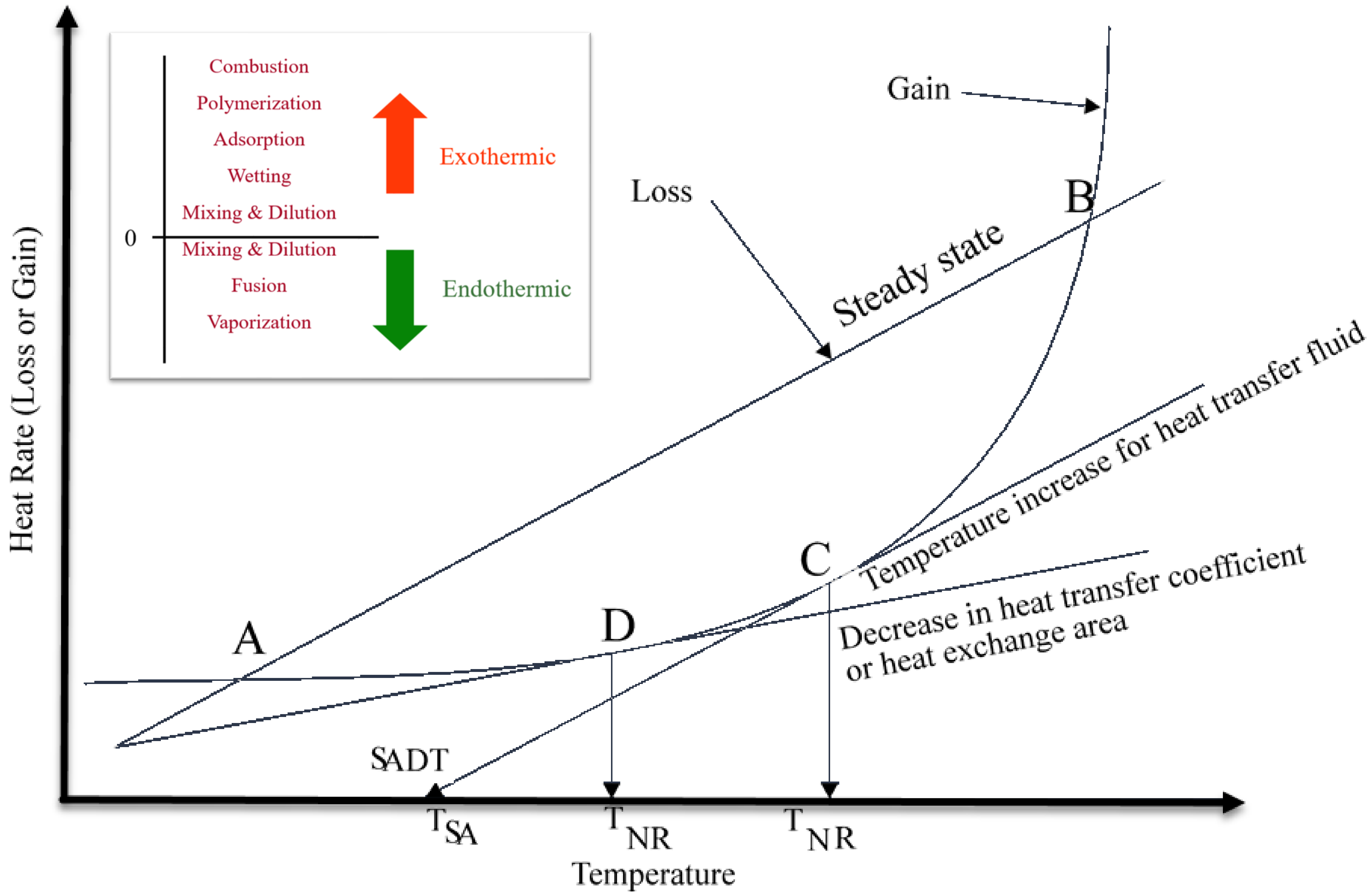
$$\delta_c = \frac{K+1}{e\left[\frac{1}{B_{i\infty}} + \frac{1}{B_i}\right]}$$

Kamenetskii:

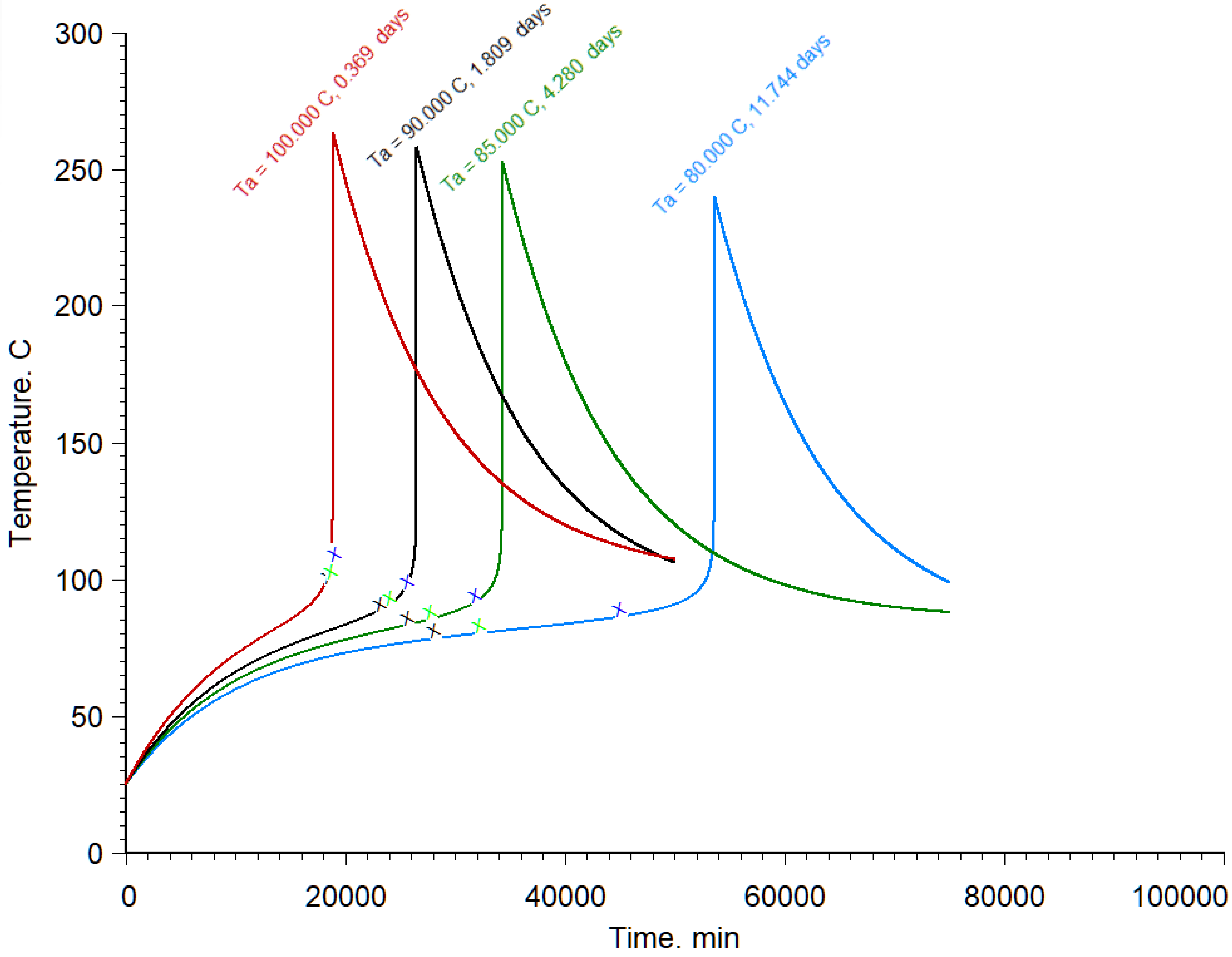
$$T_{SA}^2 = \underbrace{c_{vT}\rho_T\frac{r^2}{\lambda_T\delta_c}}_{\text{Time Constant}} \times E \times q(T_{SA})$$

Geometry or shape	K	$B_{i,\infty}$
Infinite slab	0	2.39
Infinite cylinder	1	2.72
Sphere	2	3.01
Right cylinder ($l = d$)	1.78	2.72
Finite cylinder ($l > d$) with heat loss at both ends	$1 + 0.78(d/l)^2$	2.72
Finite cylinder ($l > d$) with heat loss at one end	$1 + 0.195(d/l)^2$	2.72
Finite cylinder ($d > l$) with heat loss at both ends	$-0.12 + 1.9(l/d)^2$	2.72
Cube	1.52	2.72
Box	$0.825\,[1.067 + (x/y)^2 + (x/z)^2] - 1$	2.72

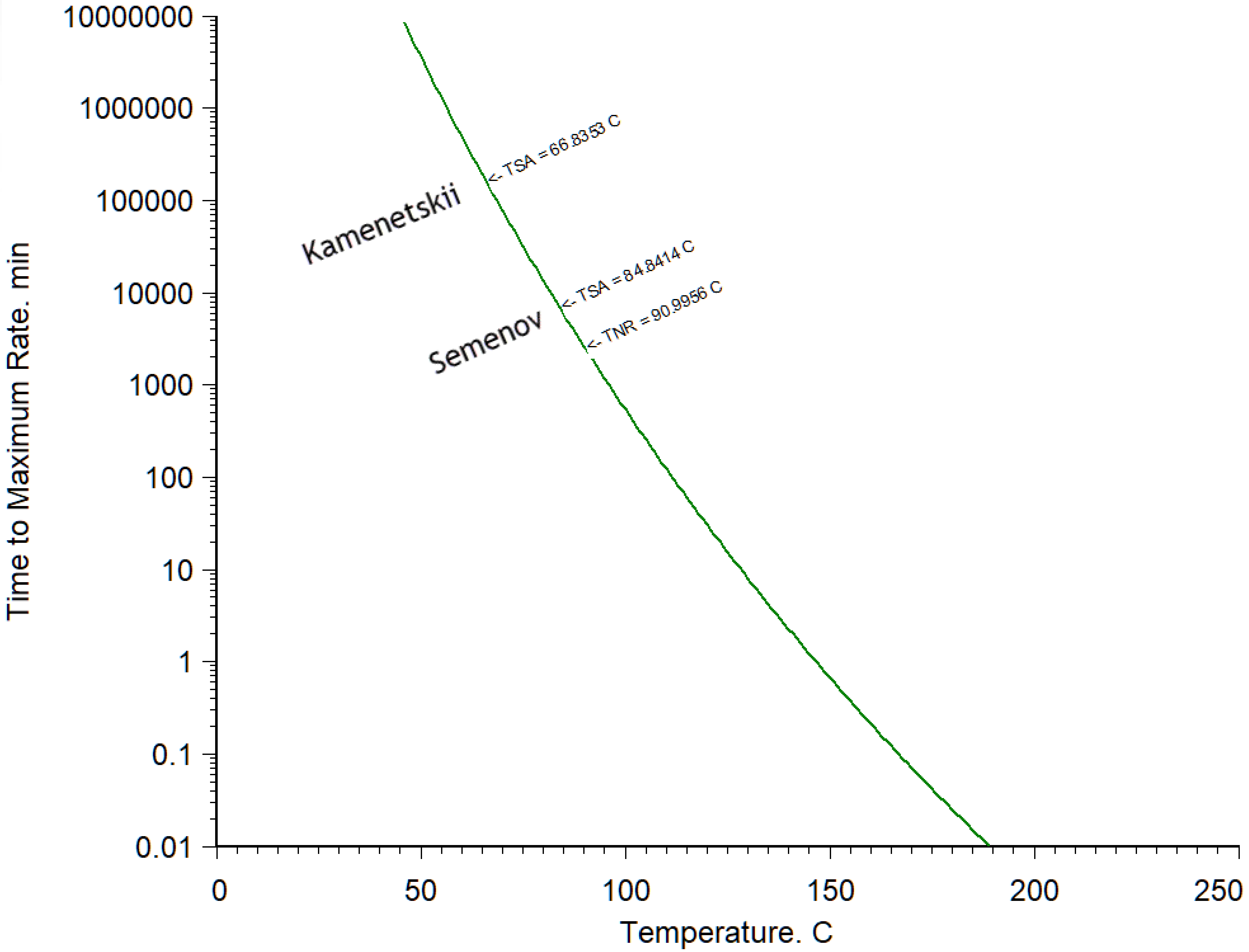
T_{NR} is the absolute maximum safe operating limit



SuperChems Expert T_{SA} or SADT estimates for 20 % di-t-butyl peroxide in toluene



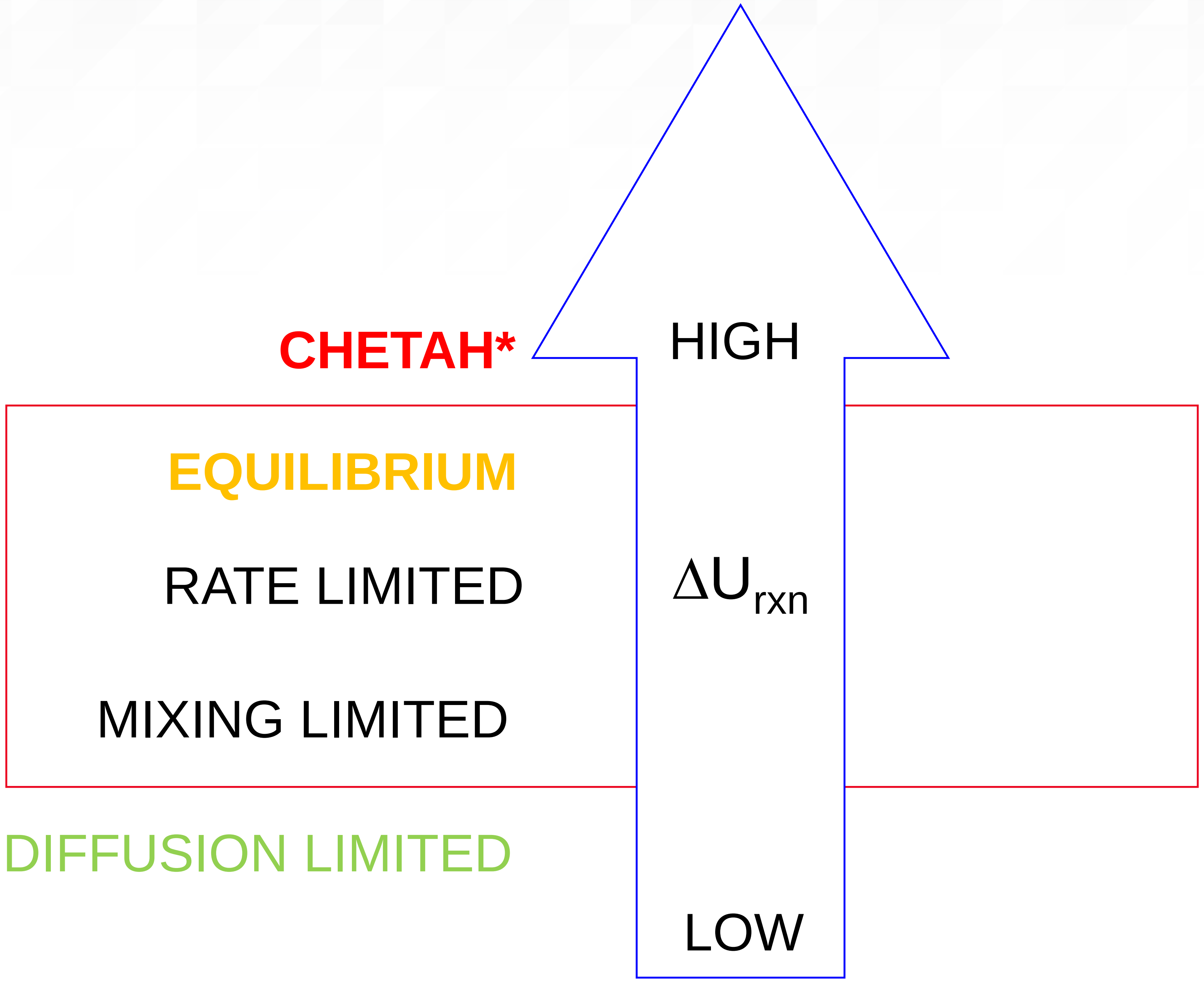
Quick estimates for t_{MR}, T_{NR}, and T_{SA} for 20 % di-t-butyl peroxide in toluene using SuperChems Expert



Detailed kinetic models can be used for thermal stability and pressure relief systems evaluations

- Direct scaleup vs. detailed kinetic modeling
- 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 proceed
- 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

Chemical equilibrium can provide insight into the potential hazards of many different types of chemical reactions



CHETAH*

EQUILIBRIUM

RATE LIMITED

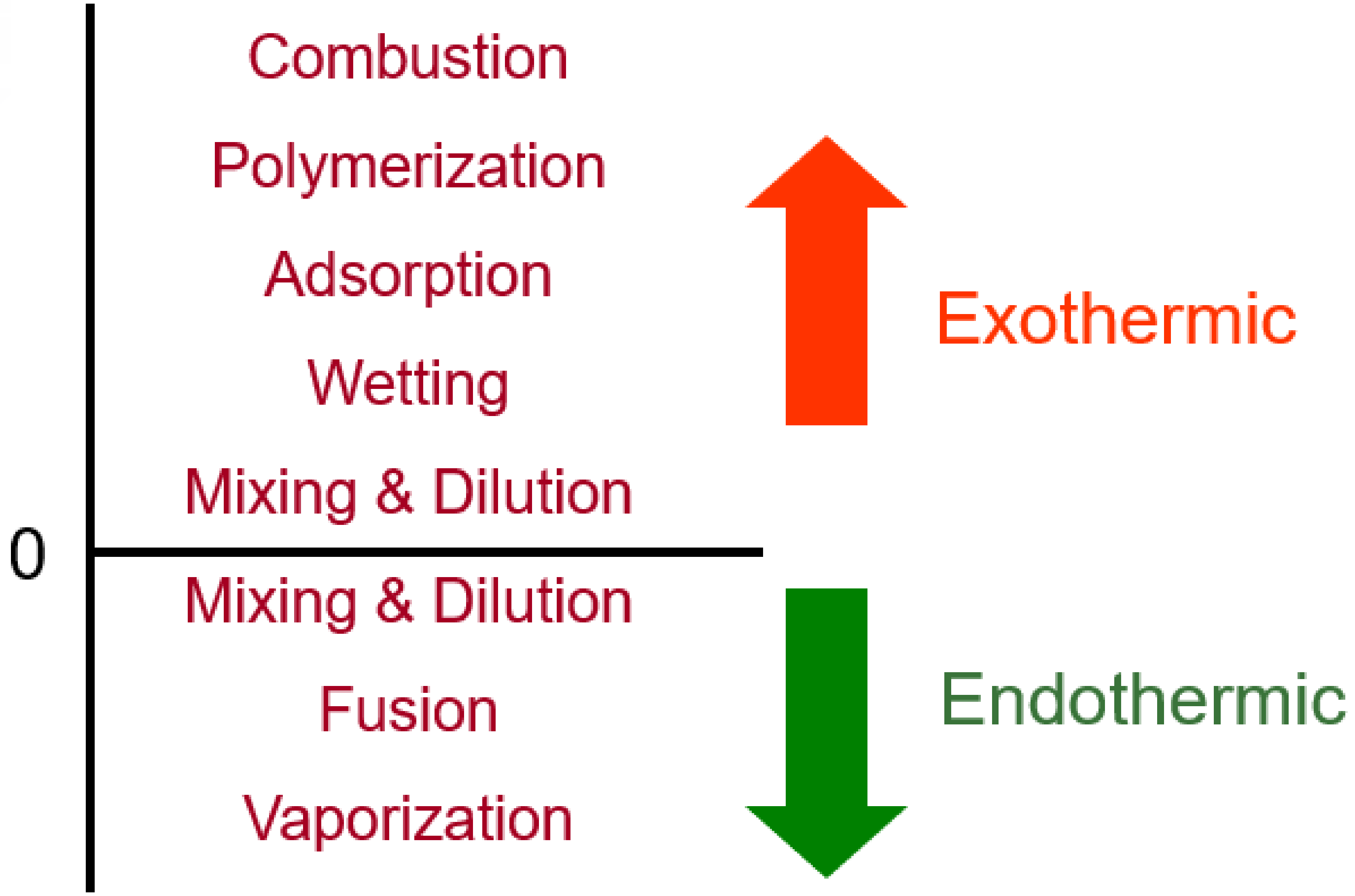
MIXING LIMITED

DIFFUSION LIMITED

HIGH

ΔU_{rxn}

LOW



Combustion

Polymerization

Adsorption

Wetting

Mixing & Dilution

0

Mixing & Dilution

Fusion

Vaporization

Exothermic

Endothermic

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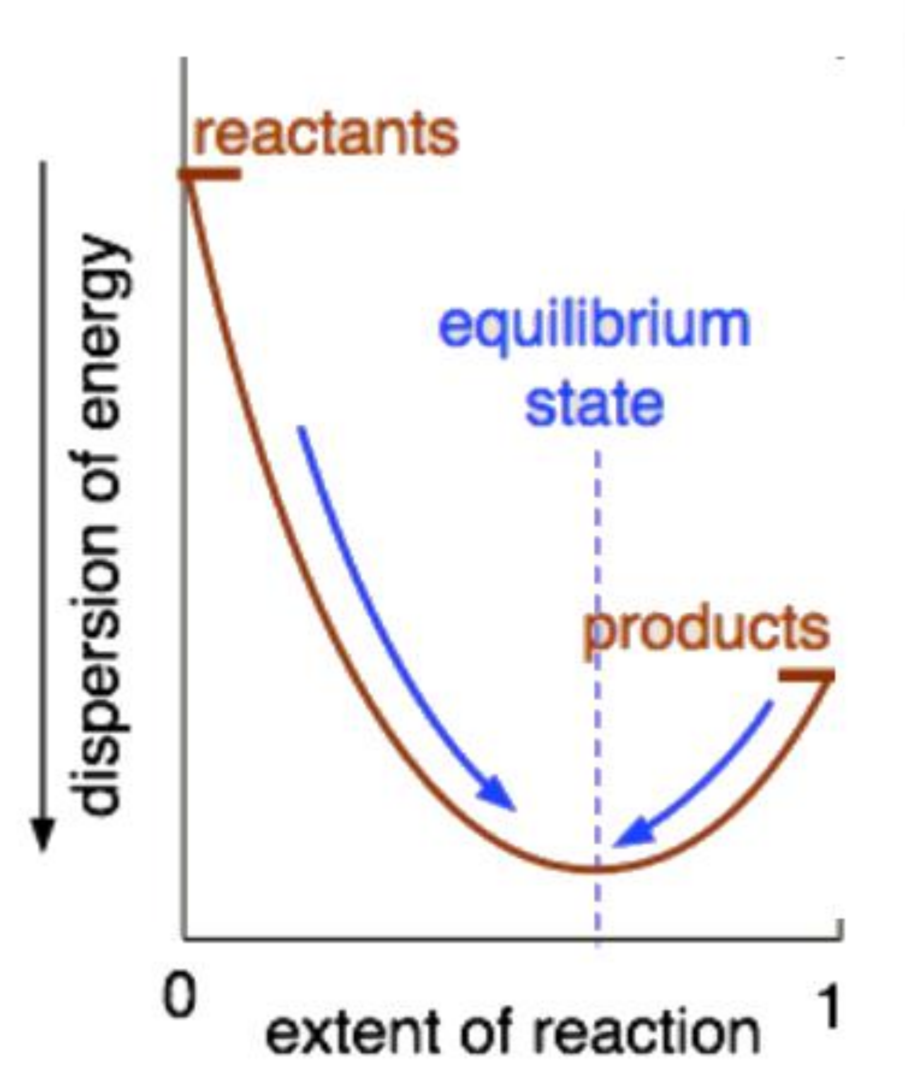
* See E. S. Shanley and G. A. Melhem, "A review of ASTM CHETAH 7.0 hazard evaluation criteria", Journal of Loss Prevention in the Process Industries, Vol. 8, No. 5, Pages 261-264, 1995

Direct minimization of the Gibbs free energy is the most effective method for calculating chemical equilibrium

- Can be used for multiphase systems (Solids, Liquids, Vapor)
- Can be constrained using limited measurements to aid in the development of reaction stoichiometry
- Can be used to screen the hazard potential of chemical reactions
- Requires an atom matrix
- Requires a large selection of potential reaction products
- Requires thermodynamic properties
- Difficult to solve for multiphase systems
- Equilibrium states are often flat and require accurate numerics



A reaction that is thermodynamically possible but lacks a rapid mechanism is said to be “*kinetically limited*”

$$\text{Reactants} \underset{k_r}{\overset{k_f}{\leftarrow\rightarrow}} \text{Products}$$

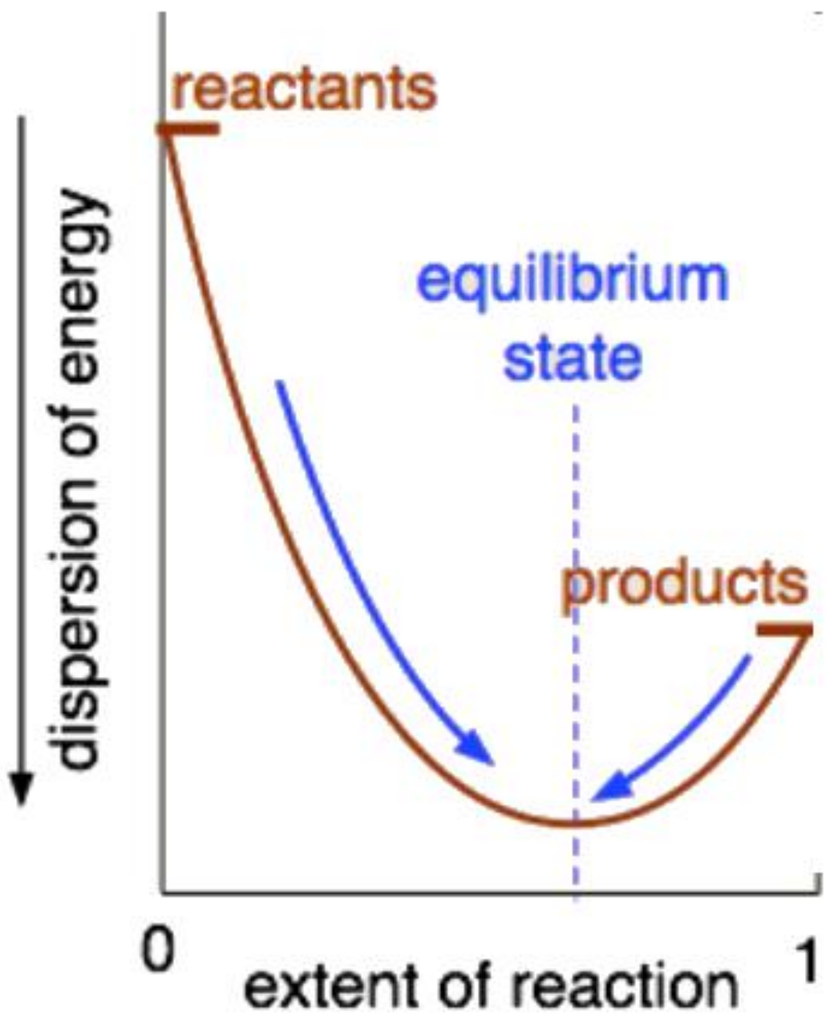
Many factors can drive a chemical reaction in either direction

$$K_{eq} = k_f / k_r$$

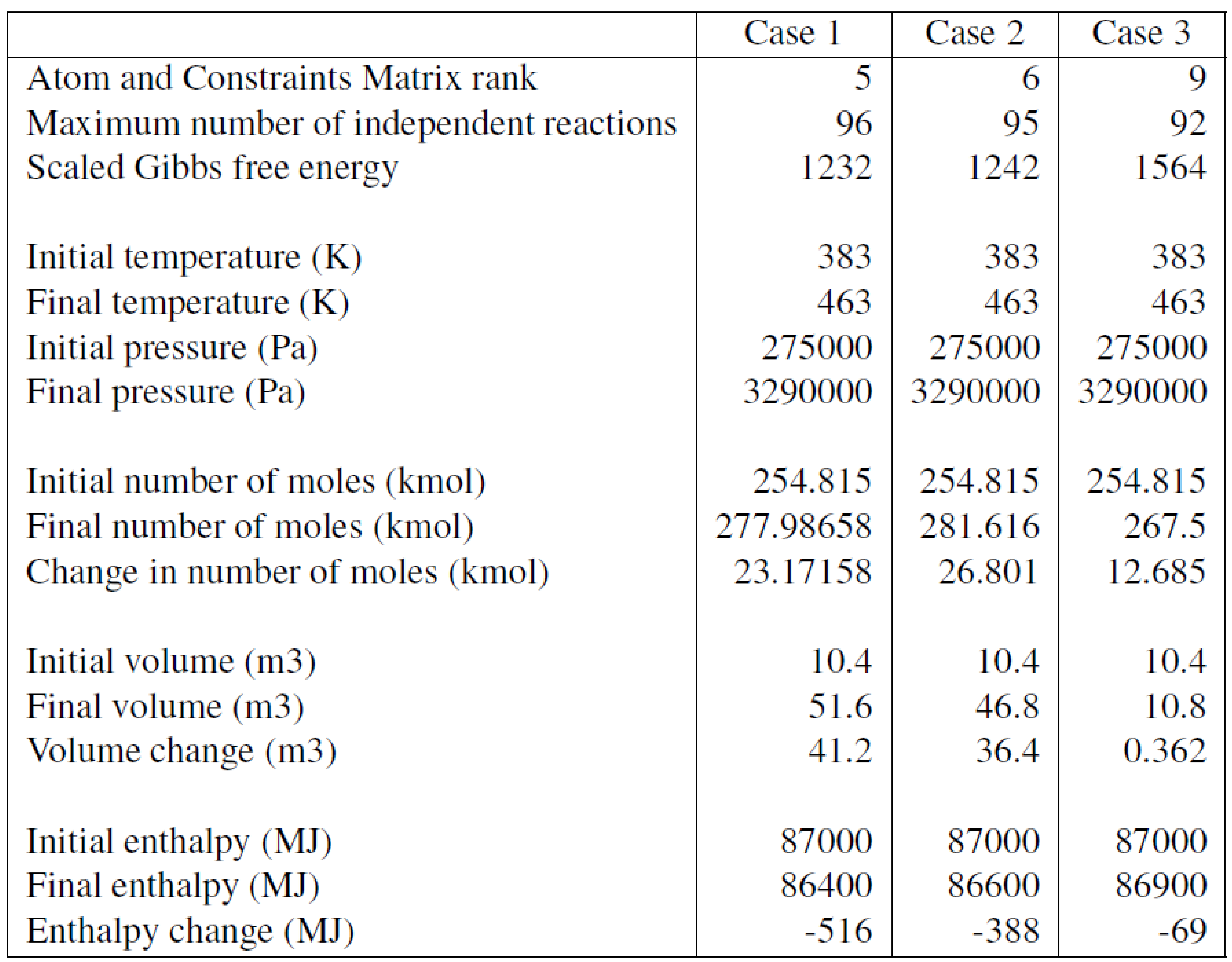
Quantity of Interest	Question	Methods
Degree of conversion	How complete is the reaction?	Thermochemistry Theoretical
Speed of conversion	How fast is the reaction?	Kinetics Measurements
Identity of components	What is the composition?	Equilibrium Constraints Measurements

Use of chemical equilibrium tools such as those provided in SuperChems Expert can speed up the development of reaction models

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

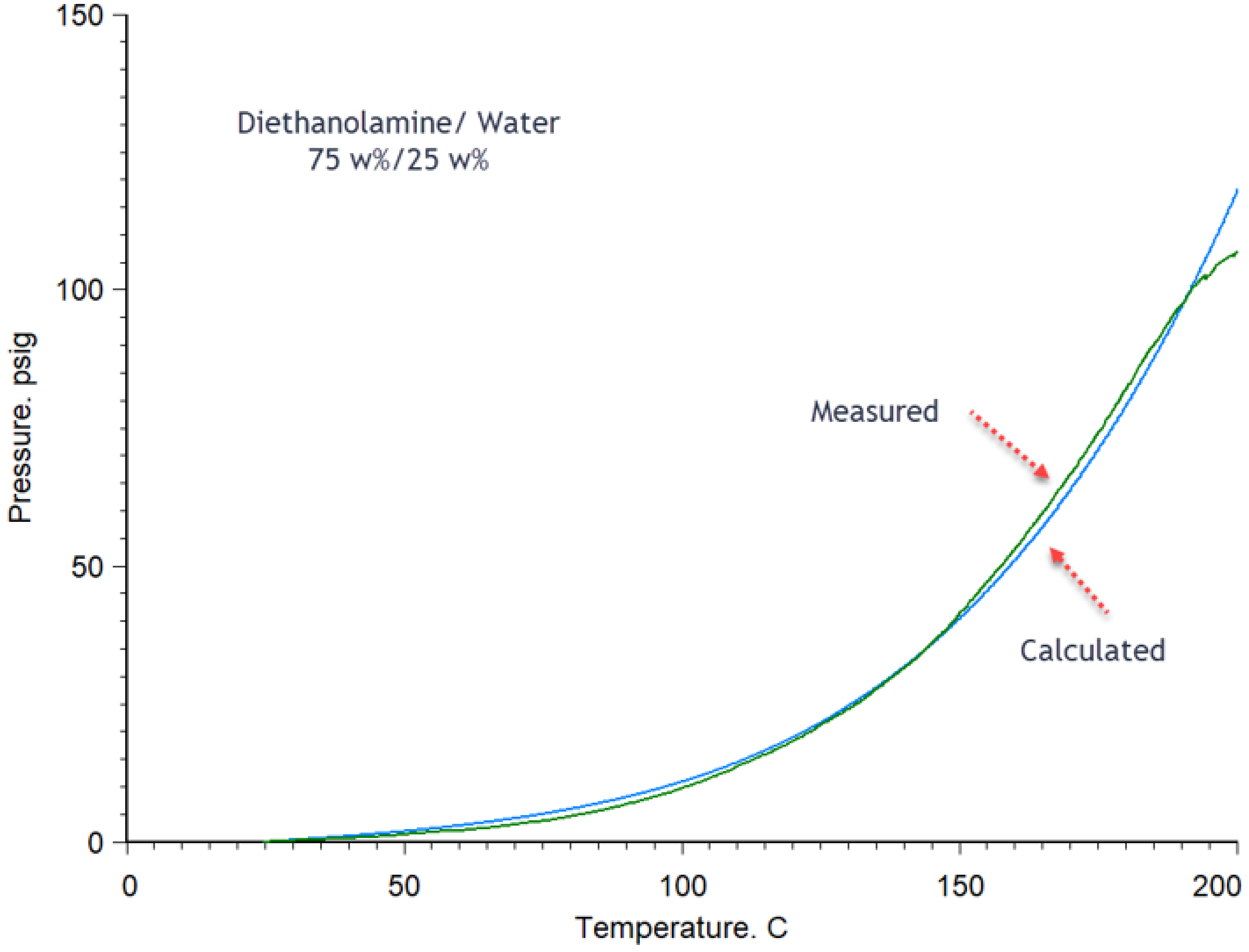


Development of reaction stoichiometry and rates requires expert skills and some understanding of the chemistry involved



	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

Stoichiometry drives vapor/liquid equilibrium and flow rate estimates



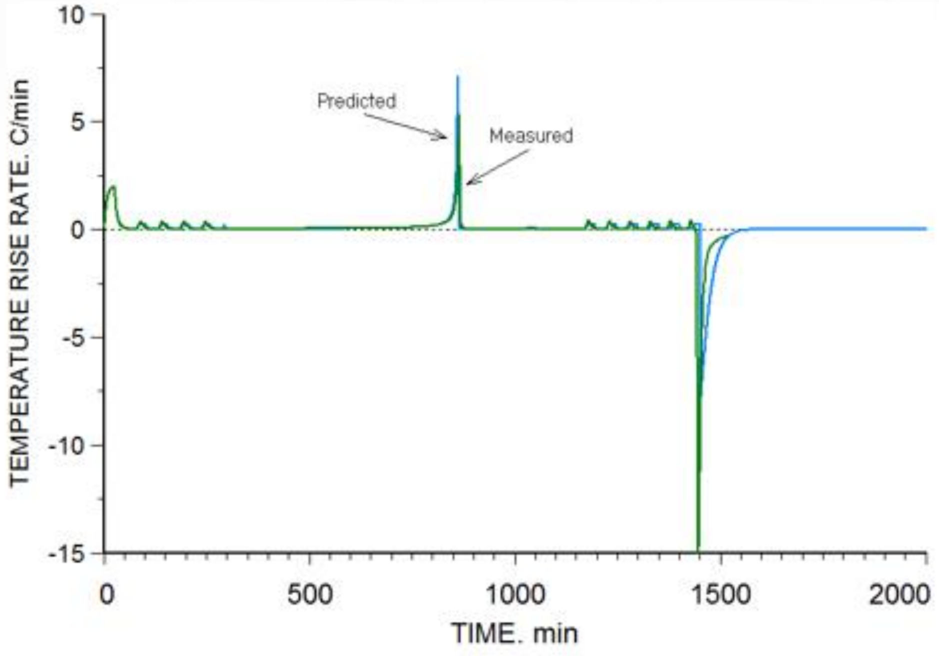
In order to develop a valid detailed kinetic model, five indicators must be demonstrated to have good fits

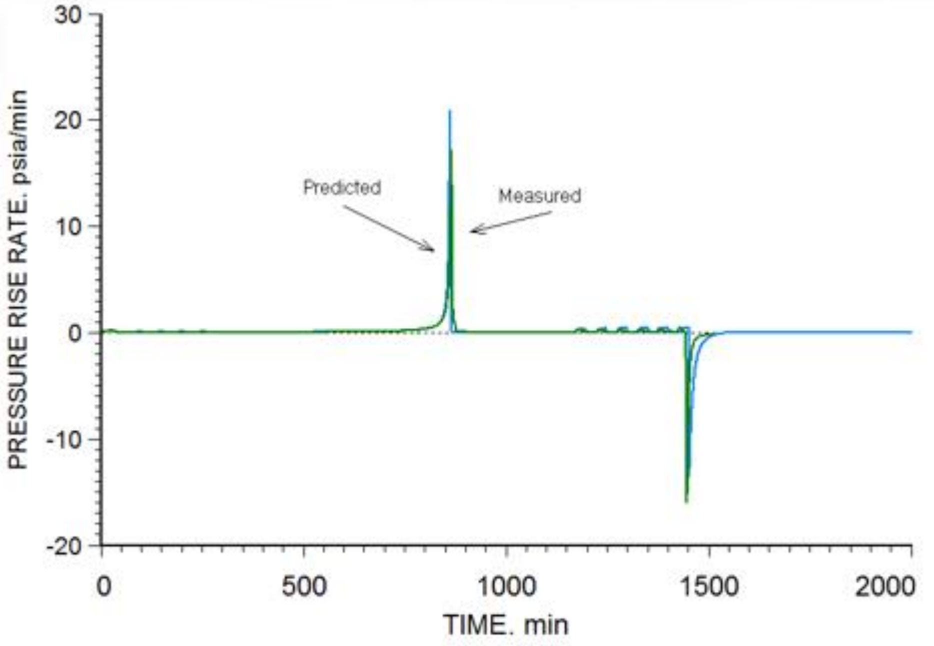
- Temperature vs. time: This should include the heat-wait-search portion of the calorimetry test or the constant heat ramp portion of the test
- Pressure vs. time: This should include the heat-wait-search portion of the calorimetry test or the constant heat ramp portion of the test
- Pressure vs. temperature: 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

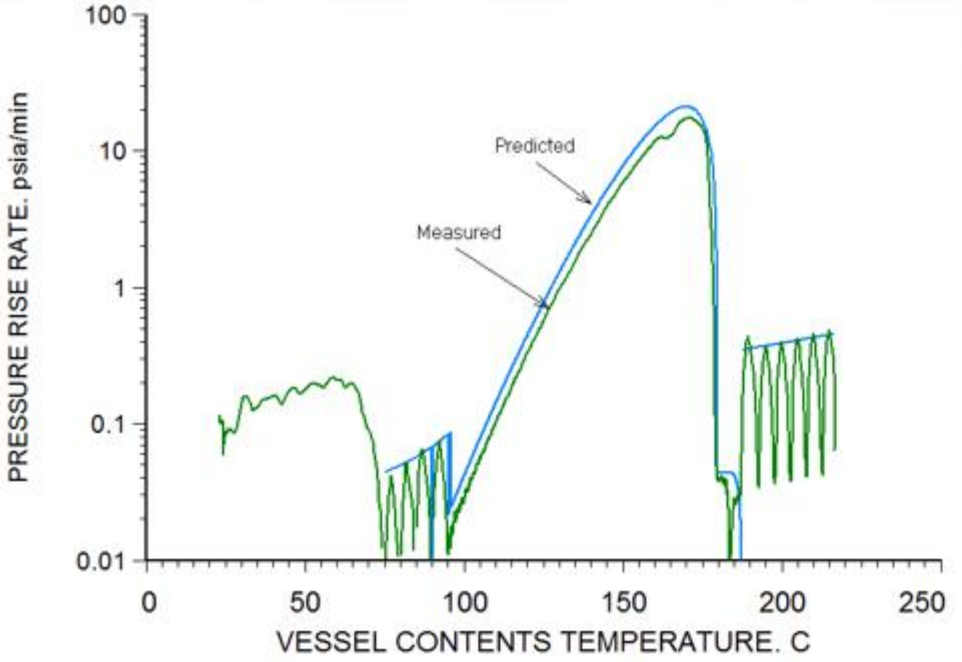
In order to develop a valid kinetic model, five indicators must be demonstrated to have good fits (continued)

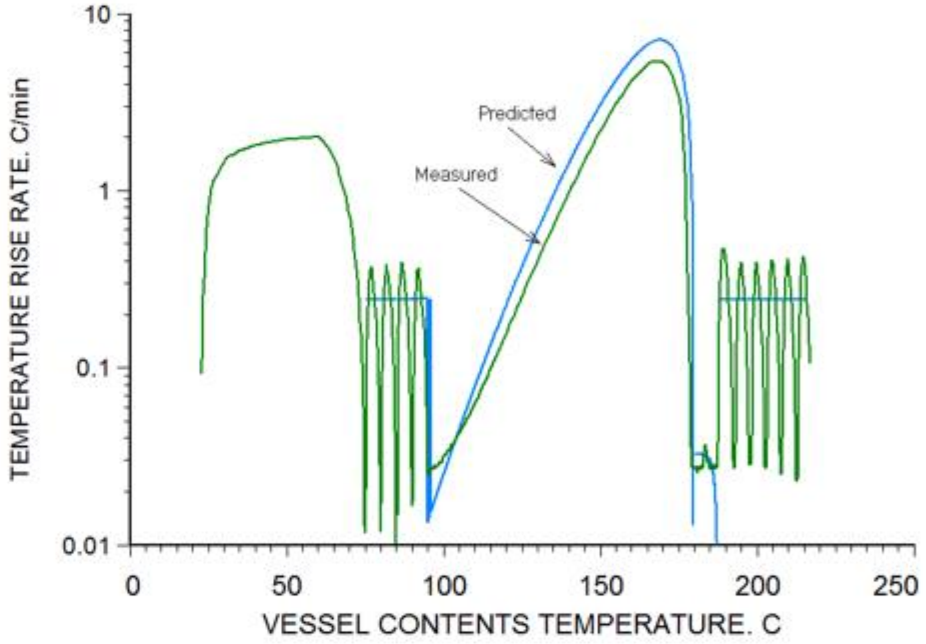
- dT/dt vs. time: This is used to also show the goodness of fit for the cool down portion of the test. Often, a logarithmic plot of dT/dt vs. Temperature is used
- dP/dt vs. time: This is used to also show the goodness of fit for the cool down portion of the test. A logarithmic plot of dP/dt vs. Temperature or dP/dt vs. dT/dt is also used.

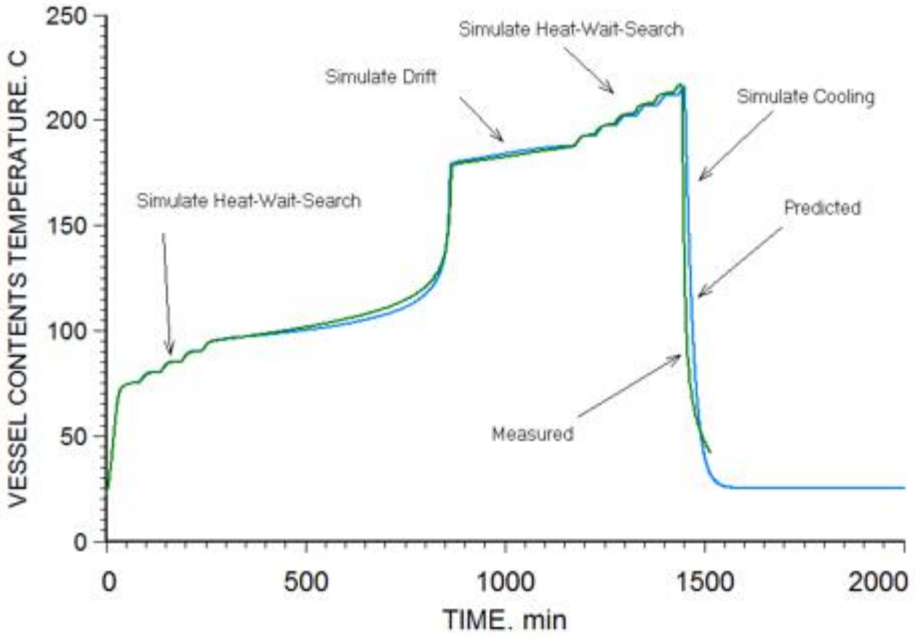
Best fit kinetic model developed using SuperChems Expert for the decomposition of 50 % dicumyl peroxide in toluene

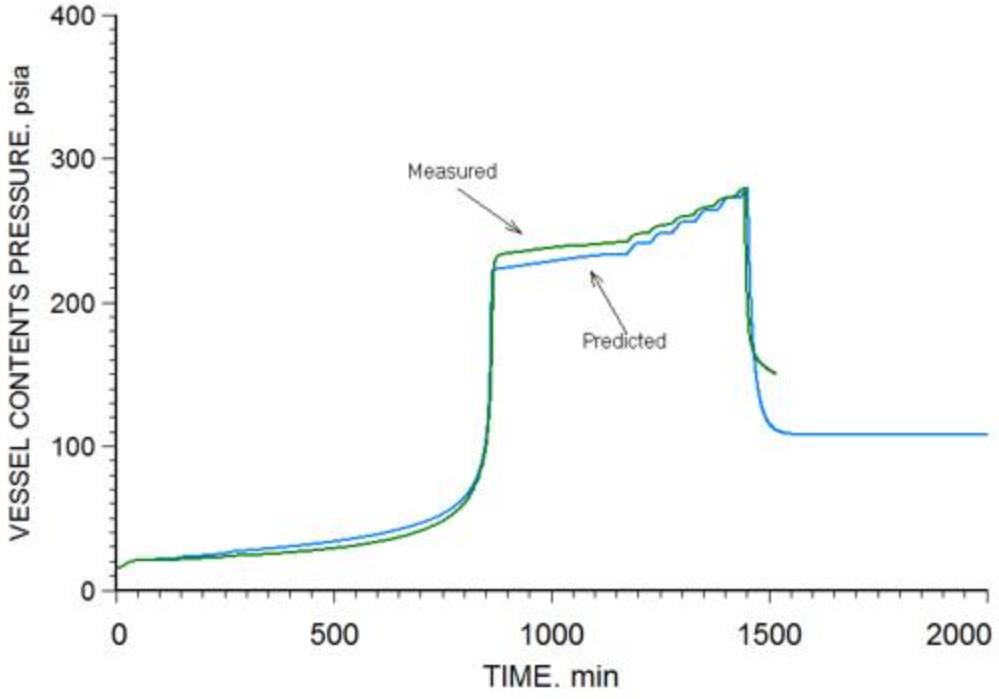




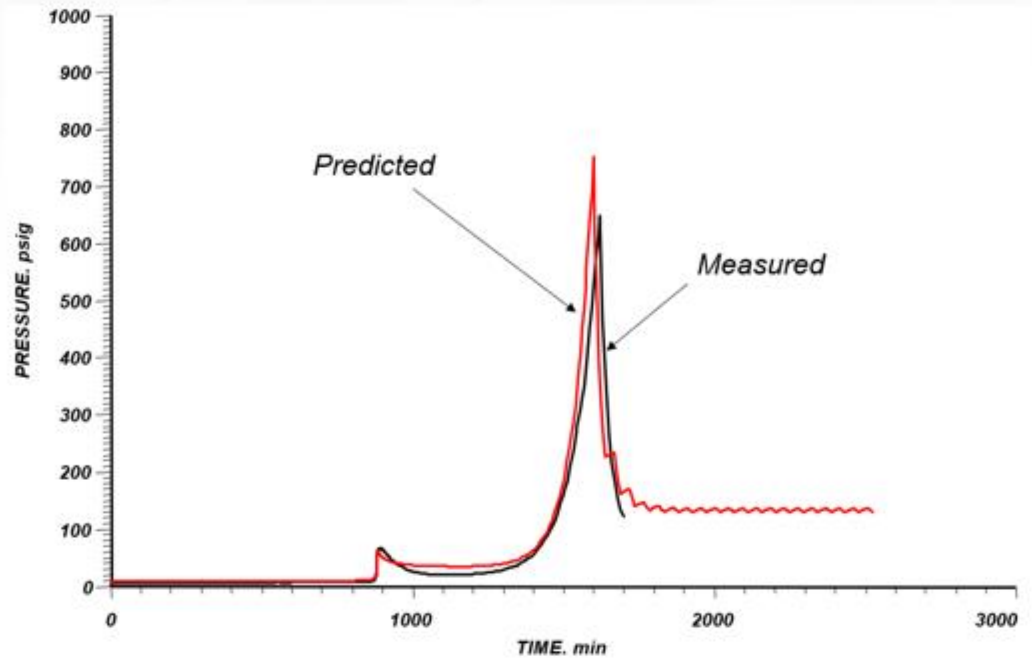


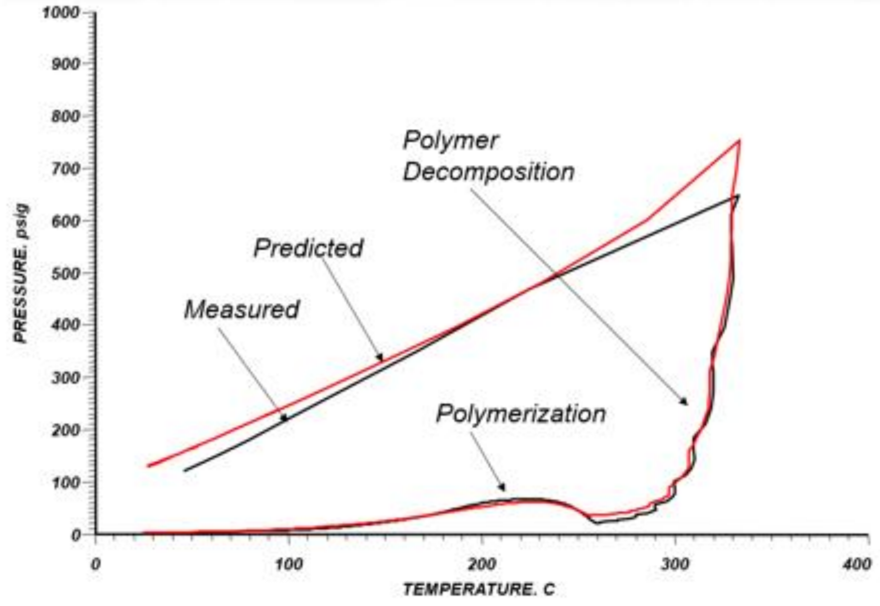


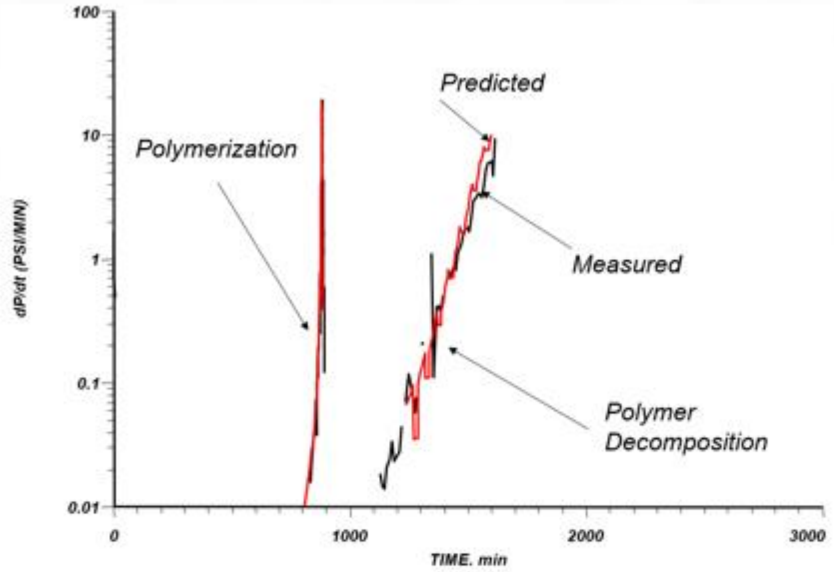


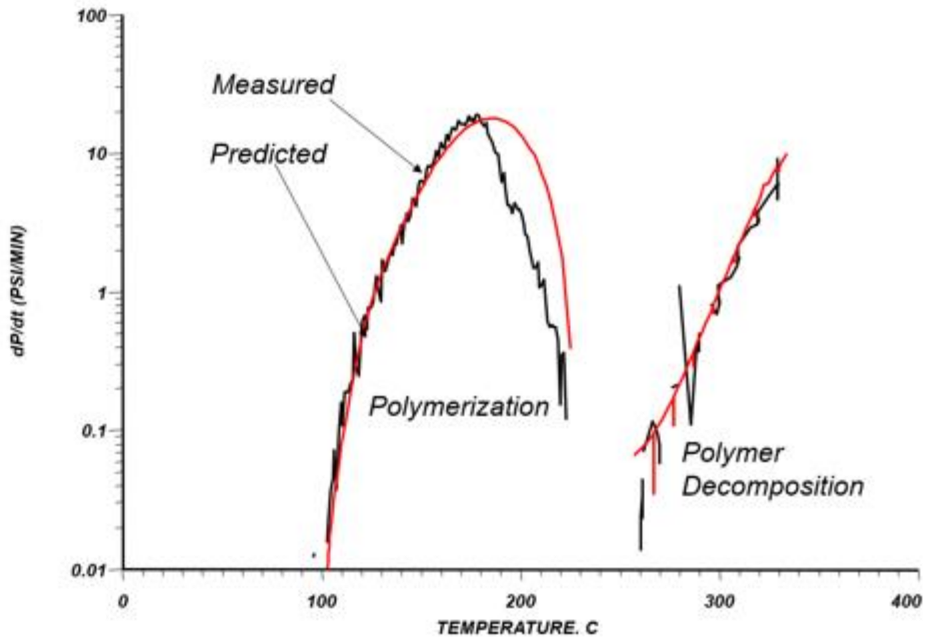


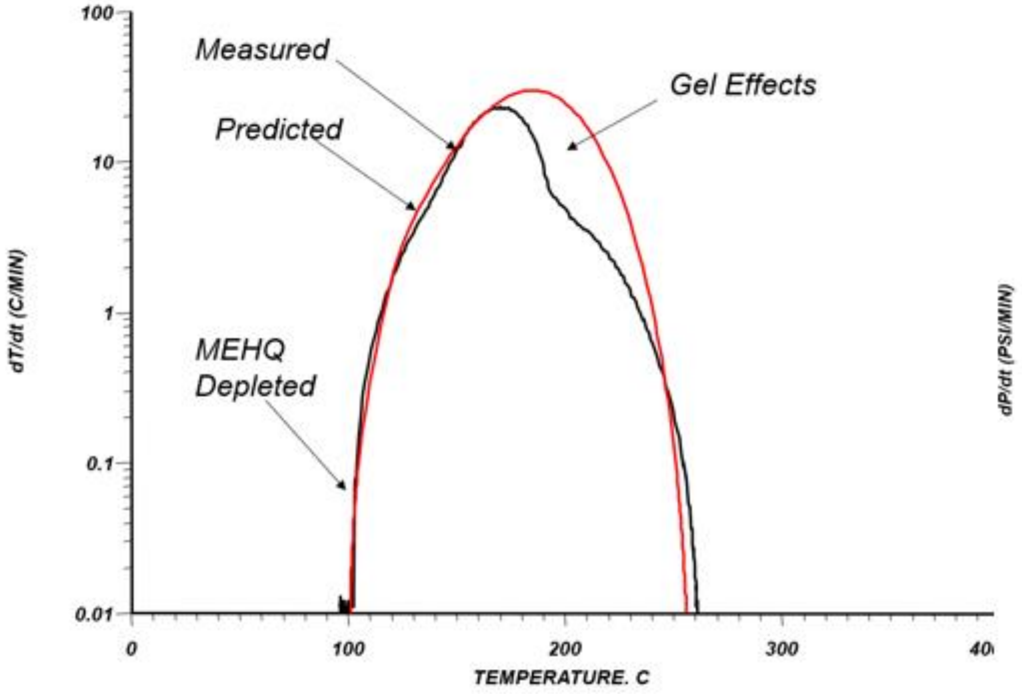
Best fit kinetic model developed for the polymerization (and polymer decomposition) of butyl acrylate inhibited with MEHQ

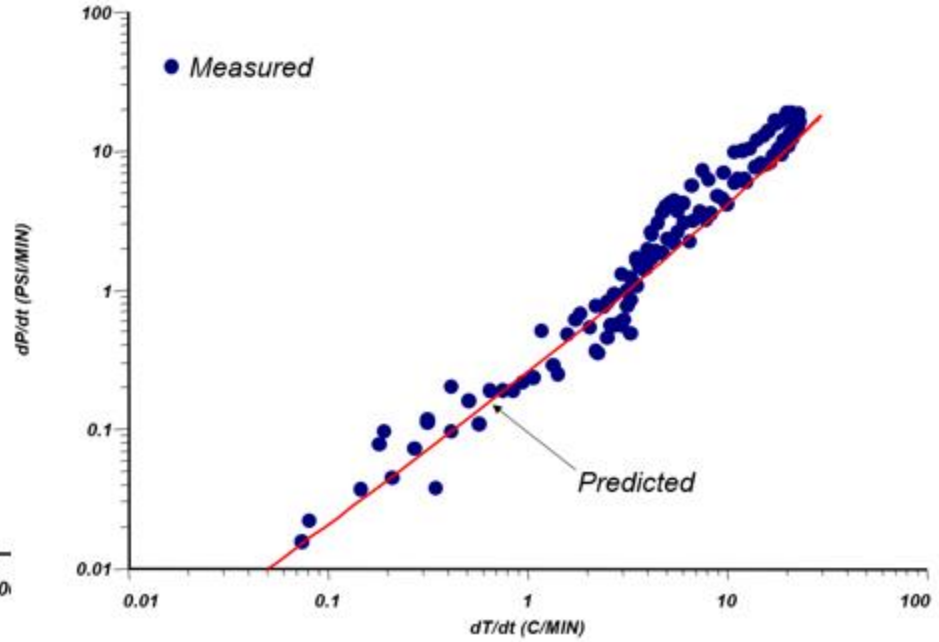




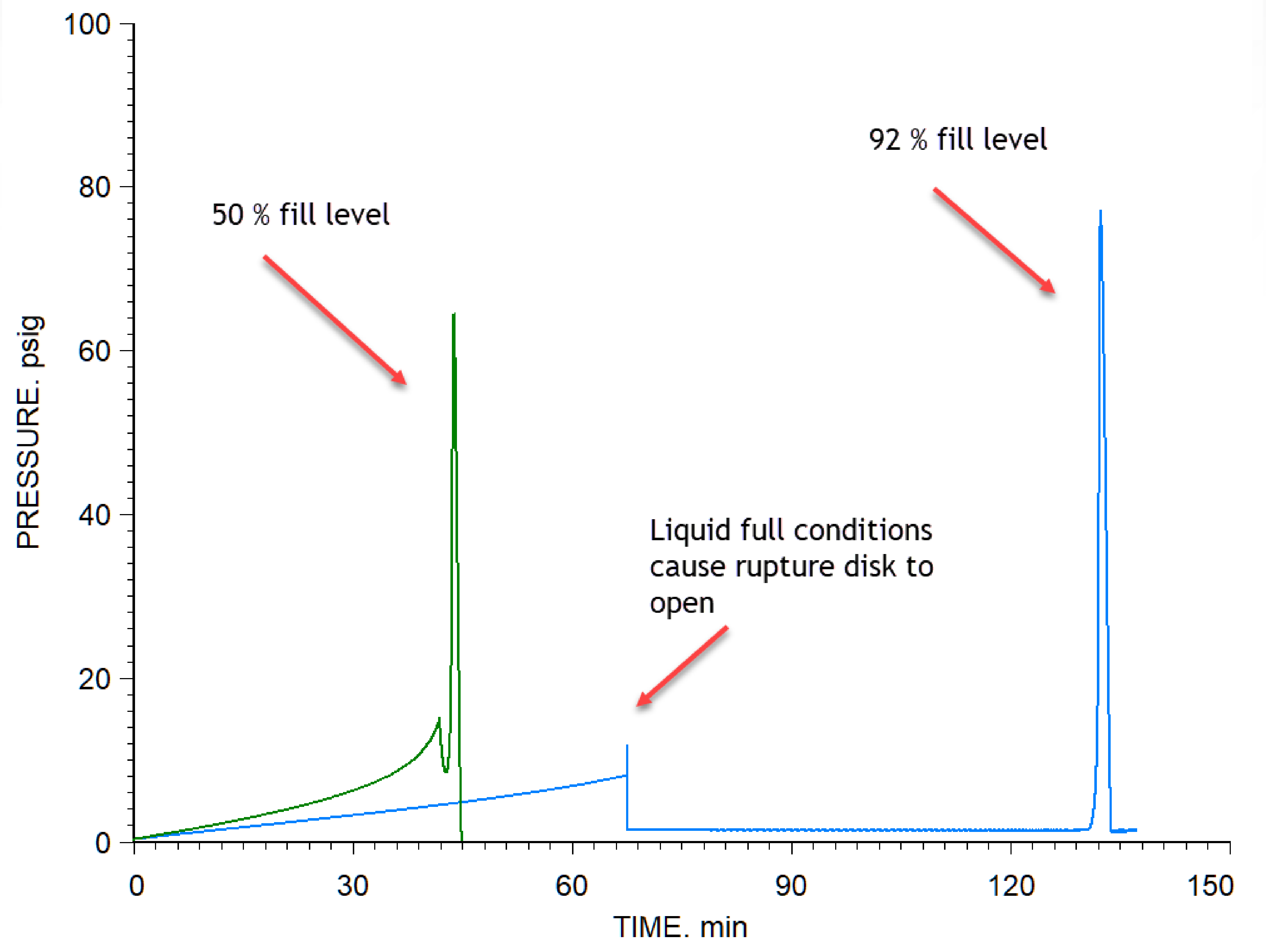








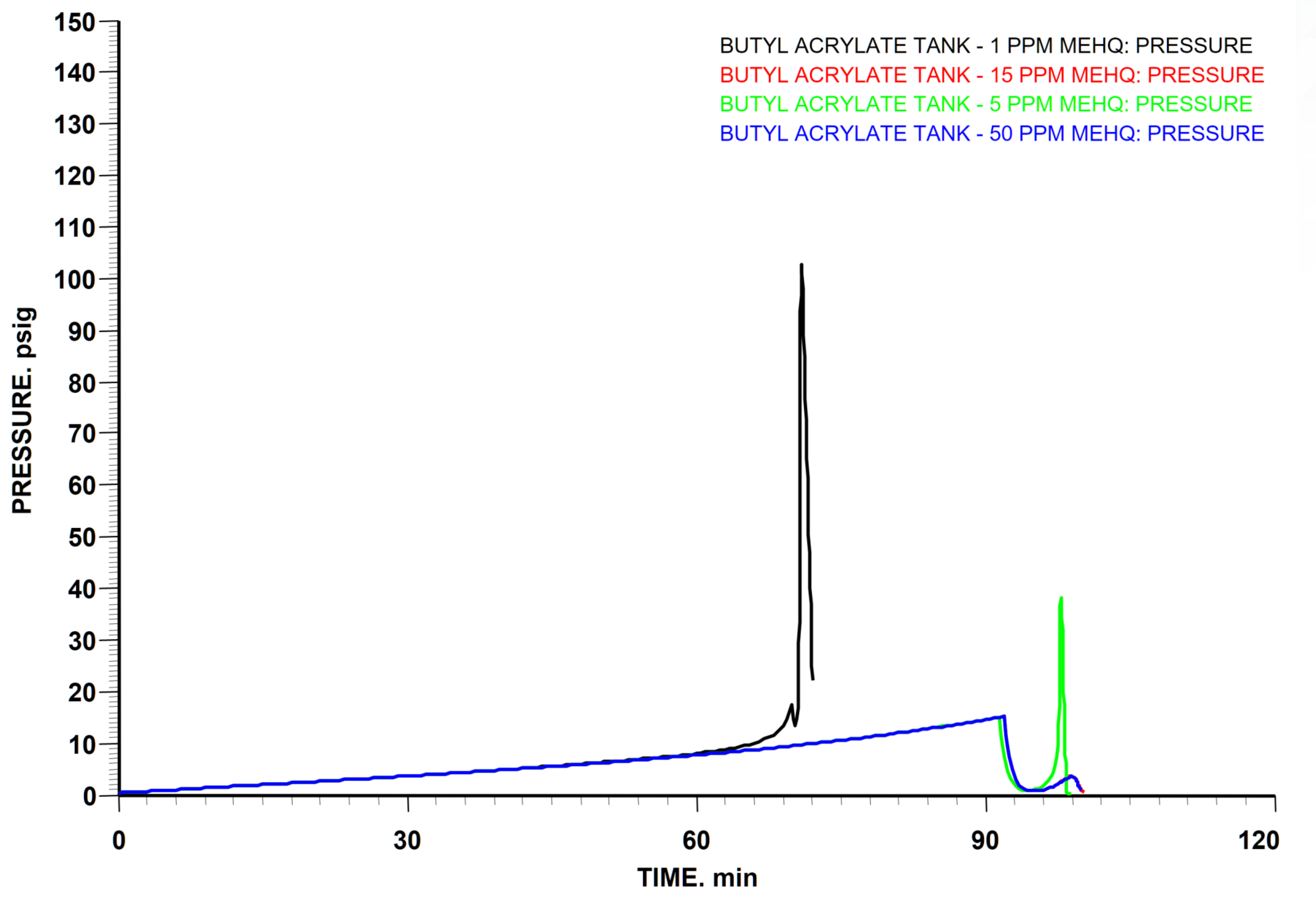
Calculated pressure-time histories for fire induced butyl acrylate runaway polymerization using SuperChems Expert



50 % fill level

92 % fill level

Liquid full conditions cause rupture disk to open



Kinetic models, simple or detailed, play an important role in chemical reaction safety

- We have developed an integrated suite of tools that can simplify and enhance the quality of chemical reaction systems evaluations for safe storage, processing, and transportation applications
- Reactivity Expert
- Reactivity data reduction and processing
- Dynamic simulation of runaway reactions

Recommended additional reading

- G. A. Melhem, *"Relief systems last line of defense, only line of defense?"*, Process Safety Progress, vol 25, No. 4, December 2006
- G. A. Melhem and Peter Howell, *"Designing Emergency Relief Systems for Runaway Reactions"*, Chemical Engineering Progress, September 2005
- G. A. Melhem, "*Calculate phase and chemical equilibria using Process Safety Office® SuperChems Expert™*", an ioMosaic Corporation white paper, March 2021.
- G. A. Melhem, "*Polymerization modeling for emergency relief systems*", an ioMosaic Corporation white paper, July 2020.
- G. A. Melhem, *"Polymerization reactions inhibitor modeling – styrene and butyl acrylate incidents case studies"*, an ioMosaic Corporation white paper, July 2020.
- G. A. Melhem, *"Quickly develop chemical interaction matrices with SuperChems"*, an ioMosaic Corporation white paper, March 2018.
- G. A. Melhem, *"Systematic evaluation of chemical reaction hazards"*, an ioMosaic Corporation white paper, August 2022.

Recommended additional reading (continued)

- G. A. Melhem, "*An advanced method for the estimation of reaction stoichiometry and rates from ARC data*", an ioMosaic Corporation white paper, August 2022.
- G. A. Melhem, S. Grenier, and L. Ding, *"Thermal stability indicators"*, an ioMosaic Corporation white paper, August 2022.
- G. A. Melhem, *"Development of kinetic models – Part I. Thermal Stability"*, an ioMosaic Corporation white paper, August 2022.
- G. A. Melhem, "*Development of kinetic models – Part II. Pressure Relief Systems*", an ioMosaic Corporation white paper, August 2022.
- G. A. Melhem, *"Advanced pressure relief design using computer simulation"*, an ioMosaic Corporation white paper, August 2022.

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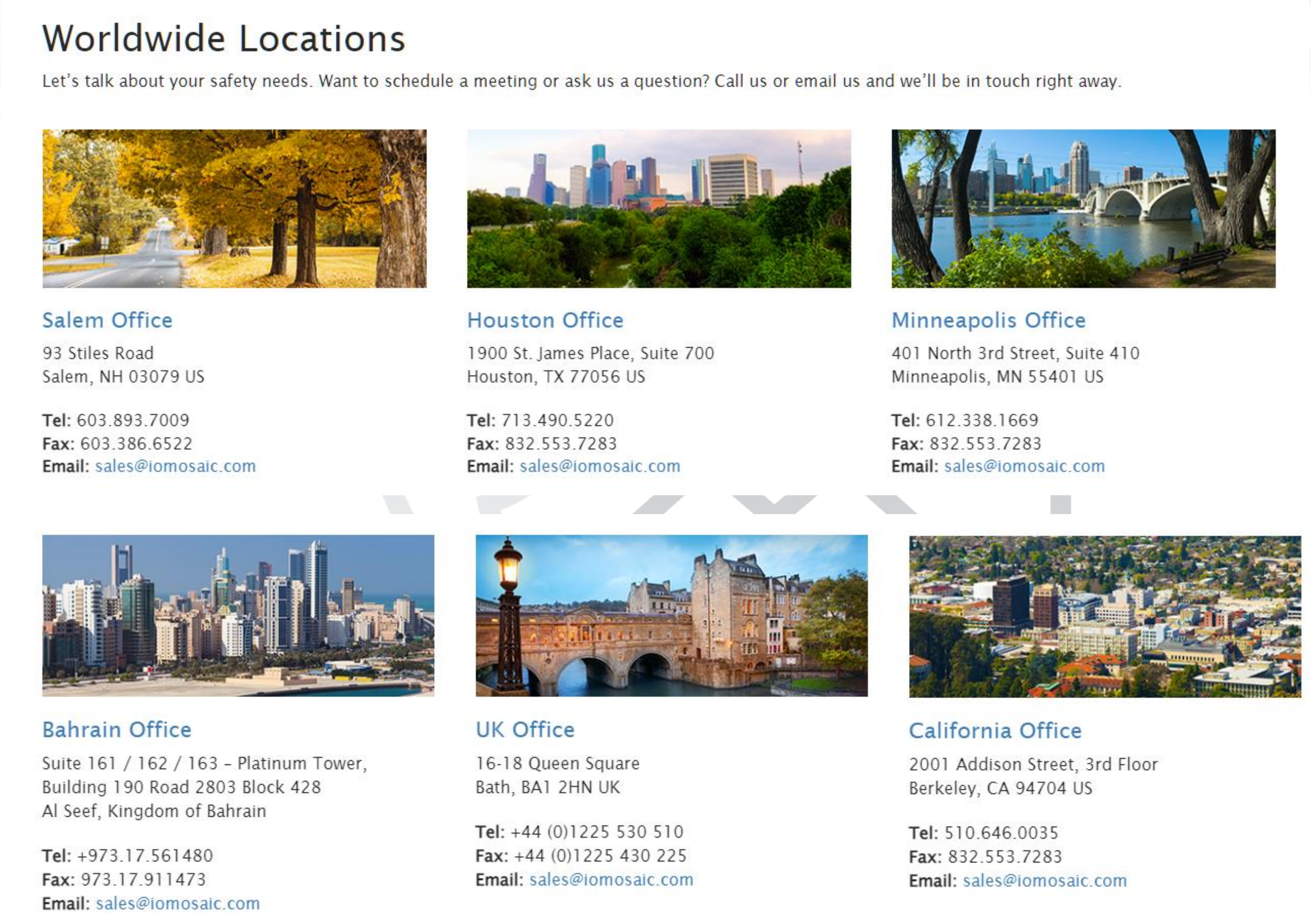

Worldwide Locations

Let's talk about your safety needs. Want to schedule a meeting or ask us a question? Call us or email us and we'll be in touch right away.

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About ioMosaic Corporation

Through innovation and dedication to continual improvement, ioMosaic has become a leading provider of integrated process safety and risk management solutions. ioMosaic has expertise in a wide variety of areas, including pressure relief systems design, process safety management, expert litigation support, laboratory services, training, and software development.

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.

For more information on ioMosaic, please visit: **www.ioMosaic.com**