Determination of SADTs Using Accelerating Rate Calorimeter

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Abstract

Safe storage, proper handling, and dependable transport of self-reactive substances are fundamental operations required in the chemical process industries. One of the key parameters used to assess the extent of a substance's reactivity is its self-accelerating decomposition temperature (SADT). Various methods for estimating the SADTs have been well documented, including the "Recommendations on the Transport of Dangerous Goods: Manual of Tests and Criteria" by the United Nations. In this paper, using the Accelerating Rate Calorimeter (ARC) to assess SADT is the primary focus. Styrene polymerization and its applicable inhibitor effectiveness, including loss of inhibitor, are evaluated. Presented as a case study, a detailed kinetic model is developed illustrating the ability and flexibility to calculate the SADTs for any package sizes, shape and configurations. Complete simulations of time to reactions thermal runaway for selected DOT storage and transport vehicle are also included.

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1 Introduction

A reactive chemical which decomposes exothermally when held in a container will either come to a thermal equilibrium or self-heat, depending on the heat generation rate and heat loss rate of the system. Given that heat generation rate is exponential to temperature and heat loss rate is linear to the temperature[1], an increase in temperature will result in a heat accumulation, potentially leading to thermal runaway and possible explosion. According to The United Nations Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria[2], a self-accelerating decomposition temperature (SADT) is the lowest ambient air temperature at which a self-reactive substance undergoes an exothermic reaction in a specified package in a period of seven days or less. The same sample and package must be able to survive for seven days at a temperature within 6°C of the temperature at which the reaction occurs. SADT of self-reactive substance is determined to decide the safe storage and transportation temperatures in a specified package. Values are determined on the assumption that the substance will only be subjected to a maximum of 55°C for a brief period any day of storage or transportation[2]. All substances having SADT temperature of 55°C or less, should be subjected to a controlled environment for storage and transport[3]. There are four test methods recommended by the United Nations (UN) for SADT determination, which mainly differ in measuring techniques and are listed below[3]:

1. United States SADT test (H1): Commercial package is tested in an isothermal oven to determine the temperature at which test sample goes to self-accelerated decomposition which damages the package and the temperature at which the package survive. The difference of temperature between survival and damage should be less than 6°C over a period of seven days.
2. Adiabatic storage test (H2): This method determines the heat generation of reactive substance as a function of temperature. A sample of 1.1 liter is taken into Dewar flask (volume of 1.5 liter), which is kept inside an oven with controls to maintain the temperature around the Dewar equal to sample, to maintain adiabaticity. A temperature of no return is calculated from the heat generation rate and the heat loss rate of a specific package (cooling curve). The benefit of this method is that the test results could be applied to any size and shape of the package.
3. Isothermal storage test (H3): This method determines the heat generation of reactive substance with respect to time at various temperatures (heat flow measurement). SADT is calculated from heat generation rate curve generated from measured data is compared with heat loss rate curve of package.
4. Heat accumulation storage test (H4): This method depends on the choice of an appropriate Dewar vessel with a similar heat flow per unit of mass to the surroundings as in the case of commercial package and uses around 400 ml sample.

The United States SADT method is the only method that is done with commercial scale packages, which results in high cost and of high potential of hazards related to thermal runaway. Heat accumulation method comes with difficulty to find a Dewar flask with similar heat transfer characteristics of the commercial package. That is the reason adiabatic storage test and isothermal storage tests are industry preferred tests with the wide application and reliable calorimeters. The calorimetry methods involve reaction kinetic measurements with a very small sample size. SADT is then estimated by heat balance calculation. The various calorimetric techniques have been used to study the SADT including differential scanning calorimeter (DSC)[4,5], accelerating rate calorimeter (ARC)[6,7,8], Isothermal C80[8] and isothermal thermal activity monitor (TAM)[10] and Dewar test[11].

The SADT study has been carried out on many reactive substances like organic peroxides [4,5,6,7,9], asphalt-salt mix[10], propellent[12,13,14] and self-accelerating polymerization temperature (SAPT) of methyl methacrylate[15]. It is well known that polymerization is a safety concern during storage and transportation of polymerizing substances[16,17,18,19]. Large quantities of monomers are transported from small containers to trucks and railcars. Inhibitor is customarily added to prevent polymer formation and oxidative degradation during shipment and subsequent storage.

This study is primarily focused on the SADT estimation of styrene monomer. At normal ambient conditions, styrene polymerizes slowly, but can accelerate exponentially at elevated temperatures. Styrene polymerization is often initiated by heat, lack of inhibitor and dissolved oxygen, and contact with peroxides and other free-radical initiators, ionic initiators, and redox initiators. Styrene polymerization process is exothermic, releasing heat at approximately 288 BTU/lb. If the evolved heat cannot be dissipated quick enough, the temperature of the monomer will rise, which increases the rate of polymerization and, as a result, intensifies the self-heating rate. The temperature may rise to the point where the reaction becomes very rapid and self-sustaining, resulting in a thermal runaway. Depending on the storage configurations, temperatures above 65°C (149°F) are found to initiate runaway polymerizations[19].

2 Study Methodologies

Two common shipment containers are examined in this study. Table 1 summarizes the basic shipment container configuration and dimensions. Note that the 55-gallon drum is assumed and modeled in a vertical position.

Table 1: ARC Test Summary

Parameter	**55-gallon Drum**	**Railcar**
Reference	DOT 49 CFR173	DOT 111A
Material of construction	Carbon steel	316L Stainless steel
Orientation	Vertical cylindrical	Horizontal cylindrical
Heads	Flat	Elliptical 2:1
Diameter, in	22½	118.92
Length, in	35¼	567.60
Wall thickness, in	0.354	7/16
Head thickness, in	0.472	15/32
Approximate volume, gal.	55	29,000

SADT is estimated using two methods:

- Analytical method: Using accelerating rate calorimeter (ARC) based on the method initially established by Wilberforce[1] and subsequently enhanced by Fisher[6,7]. This method is used to estimate SADT of styrene for the 55-gallon drum only.
- Dynamic simulation method: applying detailed inhibitor depletion and reaction kinetic model using SuperChems™, a component of Process Safety Office®. This method is used to estimate the SADT of styrene for both the 55-gallon drum and railcar.

In all cases, 4-tertiary butylcatechol (TBC) serves as the inhibitor. TBC has been found to be an effective inhibitor for styrene. When stored at high temperature or over for a long period of time, TBC levels and effectiveness will be depleted. The rate at which the TBC concentration depletes depends almost exclusively on temperature. The derivation of TBC effectiveness model is thus a major part of the methodology discussed in this paper.

ARC Test Design

Table 2 provides a summary of the ARC test cell and material used in this study. In this study, one closed heat-wait-search (H-W-S) mode test was conducted with styrene and air as headspace. Its primary objective was to determine the onset temperature of exotherm caused by polymerization. The test was run from 50ºC to 350ºC with detection rate of

0.02ºC/min. The temperature and pressure responses were recorded, as well as the cool down temperature and pressure data once the sample reached 40ºC. The end weight of the test cell and residue were also recorded.

The onset temperature determined from the H-W-S mode test was used to establish the basis for subsequent iso-aging (isothermal) tests. Given that styrene contains 10-15ppm of TBC as inhibitor, three additional closed ARC tests were conducted with similar conditions, but with isothermal mode at temperatures below the onset obtained from the H-W-S mode test. In this case, each test was kept constant at 80ºC, 85ºC and 90ºC with exotherm sensitivity detection sensitivity of 0.005ºC/min. These tests were conducted to study the effect of induction (incubation) time on the thermal runaway. Part of the data was also used to estimate the activation energy of the polymerization reaction.

Table 2: ARC Test Summary

Key Test Parameter	**H-W-S ARC Test**	**Isothermal ARC Test**
Test cell material	Titanium	Titanium
Weight of test cell, g	10.074	10.074
Styrene, g	6.003	6.003
Headspace	Air	Air
Thermal inertia	1.42	1.42
Vessel volume, ml	9.1	9.1
Start temperature, ºC	50	80, 85, 90
End temperature, ºC	350	End of exotherm
Exotherm sensitivity, ºC/min	0.02	0.005

SADT Determination by Wilberforce method

Figure 1 illustrate the basic concept of the relationship between the heat generation rate and heat loss rate of a system. In general, a reactive chemical which decomposes exothermally when held in a container will either come to a thermal equilibrium or self-heat, depending on the balance of these heating/cooling rates. Given that heat generation rate is exponential to temperature and heat loss rate is linear to the temperature[1], an increase in temperature will result in a heat accumulation, potentially leading to thermal runaway and possible explosion. The point at thermal equilibrium indicates a temperature of no return (T_{NR}). In order to obtain the SADT, the objective of this method is to estimate the time constant and the T_{NR}.

The ARC test with heat-wait-search mode proposed in this study measured onset temperature and heat rates as function temperature. Isothermal tests provided the induction time and time to maximum rate data which is used to generate the appropriate plots and properties as described by Townsend and Tou[23]. In addition to Time to Maximum Rate

(T_{MR}) versus Temperature developed from the ARC data, one key property required for SADT estimation is the activation energy.

The time constant, τ [h], for a given package is obtained according to the formula given by Wilberforce[1], as shown in Equation 1:

$$\tau = m\frac{Cp}{U(1.8)S} \qquad \text{(Eq. 1)}$$

where m is mass of sample [lb], C_p is specific heat capacity [BTU/lb/^oC], U is heat transfer coefficient of system [BTU/h/ft^2/^oF], and S is surface area [ft^2].

Once the time constant is calculated and based on the Time to Maximum Rate (T_{MR}) curve developed, the temperature of no return (T_{NR}, ^oC) can be obtained from the TMR plot.

SADT is then calculated using the estimated T_{NR} and activation energy based on the Equation 2.

$$T_{SADT} = T_{NR} - \frac{R(T_{NR}+273.15)^2}{E} \qquad \text{(Eq. 2)}$$

where T is temperature [^oC], E is activation energy [cal/gmol], U is the universal gas constant [1.987 cal/gmol/K].

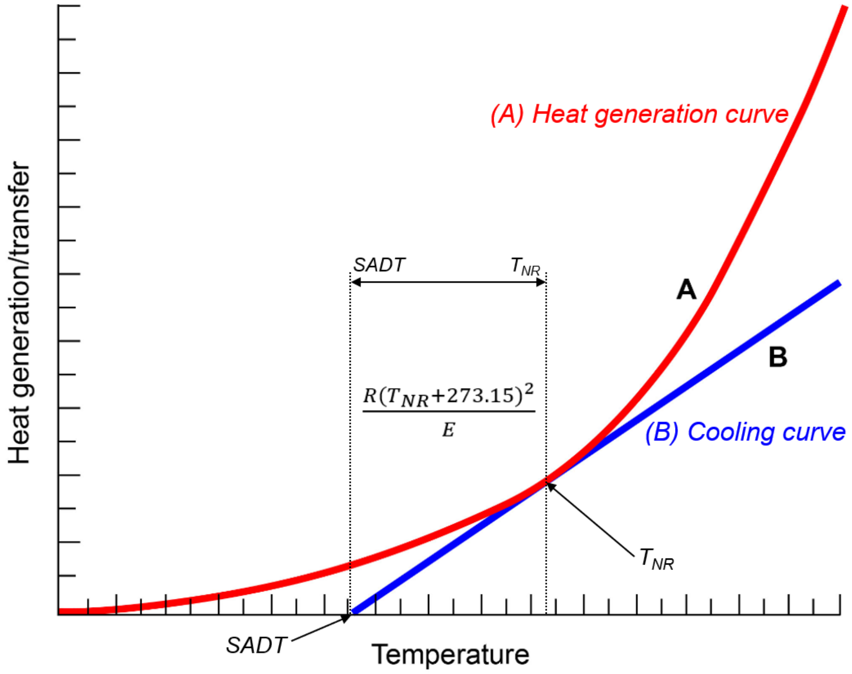

Figure 1: Thermal Equilibrium, Illustrating Relationship between T_{NR} and SADT

SADT Determination by Dynamic Computer Simulation

The portion of this case study was performed using SuperChems^{TM}, a detailed dynamic simulator and a component of ioMosaic's Process Safety Office®. The program consists of various models for simulating the fluid dynamics of vessels and pipeline containing multi-phase fluids.

SADT estimation using computer simulation requires an understanding of the kinetic models of styrene polymerization and its inhibitor effectiveness. Once the kinetics are established, they can be used to simulate the equipment dynamics for equipment of any sizes and shapes at any ambient conditions, including all applicable thermal effects and heat transfer mechanisms between the fluid and its surroundings.

Thermally Initiated Polymerization of Styrene

The following kinetic rate expression published by Hui-Hamielec[24] has been well validated to account for the thermally initiated polymerization of styrene, as shown in equation 3:

$$r = A_0 e^{(A_1 S + A_2 S^2 + A_3 S^3)} C_s^{2.5} \qquad \text{(Eq. 3)}$$

$$A_0 = 1.964 \cdot 10^5 \cdot e^{\frac{-10040}{T}}$$

$$A_1 = 2.57 - 5.05 \cdot 10^{-3} \cdot T$$

$$A_2 = 9.56 - 1.76 \cdot 10^{-2} \cdot T$$

$$A_3 = -3.03 + 7.85 \cdot 10^{-3} \cdot T$$

where r is the rate of styrene polymerization [kmol/m^3-sec], A_0 is a rate constant [m^3/kmol-sec$^{2/3}$]$^{3/2}$, S is mass fraction of polystyrene, T is temperature [K], and C_s is the styrene monomer concentration [kmol/m^3].

Note that thermal decomposition of styrene polymer is also possible. When heated to elevated temperatures, polystyrene will depolymerize and decompose to form styrene monomer, dimer, trimer, toluene and small quantities of non-condensable gas[25,26,27]. The decomposition is endothermic[28] with an estimated heat of reaction of 294 BTU/lb. However, the kinetic model for polystyrene decomposition is not required for the purpose of SADT determination as decomposition would occur at much higher temperature.

TBC Inhibitor Depletion Model Development

Given that the inhibitor depletion primarily depends on temperature, temperature dependent data on the inhibitor effectiveness are needed. Manufacturers often provide some data showing the effectiveness of their inhibitors. Table 3 provides a few sample data points for the effect of TBC on the shelf life of styrene at different temperatures.

Table 3: Temperature Effect of TBC on the Shelf Life of Styrene[19]

Temperature	12 ppm TBC†	50 ppm TBC†
15.6 ºC (60ºF)	6 months	1 year
29.4 ºC (85ºF)	3 months	6 months
43.3 ºC (110ºF)	8-12 days	< 30 days

†Saturated with air

The inhibitor depletion model can be derived from the generic differential equation and Arrhenius rate expression as shown in equations 4 and 5:

$$\frac{dC}{dt} = -kC^n \qquad \text{(Eq. 4)}$$

$$k = Ae^{-\frac{E}{RT}} \qquad \text{(Eq. 5)}$$

where *dC/dt* is the rate of inhibitor depletion [ppm/s], *k* is the Arrhenius rate expression [1/s], *A* is the pre-exponential factor [1/s], *E* is the activation energy, *R* is the gas constant, *T* is temperature [K], *C* is the inhibitor concentration [ppm], and *n* is reaction order.

Assume that the depletion rate follows a first order reaction (*n=1*). Substituting *n* as *1* into equation 4 and rearranging/integrating both sides will result in an integral solution at initial (*subscript i*) and final (*subscript f*) conditions, as shown in equation 6:

$$\ln\left(\frac{C_f}{C_i}\right) = -\mathrm{k}(t_f - t_i) \qquad \text{(Eq. 6)}$$

Note that the Arrhenius rate expression, *k*, is the only unknown, which can be solved to obtain the ultimate parameters of interest: pre-exponential factor (*A*) and activation energy (*E*) based on the any pair of inhibitor temperature data. Since multiple temperature data points are provided at a given TBC concentration, the pre-exponential factor and activation energy can be obtained by plugging the applicable data points and solving the two Arrhenius rate expressions simultaneously.

Take the 12 ppm TBC data from Table 3 as an example. Pick the 60ºF as the first data point. At the initial condition when time t_i is 0, the concentration C_i is thus 12 ppm. Assume that the inhibitor completely losses its effectiveness when TBC concentration falls to 1 ppm. Therefore, at the final time t_f equal to 6 months, the final concentration C_f would be 1 ppm. Likewise, pick another temperature point and repeat the same procedure and solve for *k*. For each equation derived from a selected temperature, take a natural log on both sides of the equation. Solving the two equations simultaneously for *A* and *E* would fulfill the *k* Arrhenius rate expression, forming a complete depletion model as shown in equation 7:

$$\frac{dC}{dt} = -1.67 \cdot 10^{11}\, e^{-\frac{11888}{T}} C \qquad \text{(Eq. 7)}$$

What the TBC depletion model does is to delay the styrene from polymerizing until TBC concentration is completely depleted, falling to 1 ppm. Figures 2 and 3 illustrate the TBC depletion model integrated with the thermally initiated polymerization of styrene for one ARC experiment run. As shown in Figure 2, the temperature is kept constant (isothermally) at 80ºC, the visible reaction starts after about 18 hours. In Figure 3, a sharp pump (at 80ºC) indicates that TBC is completely depleted, losing its effectiveness. After which, the styrene polymerization model takes over.

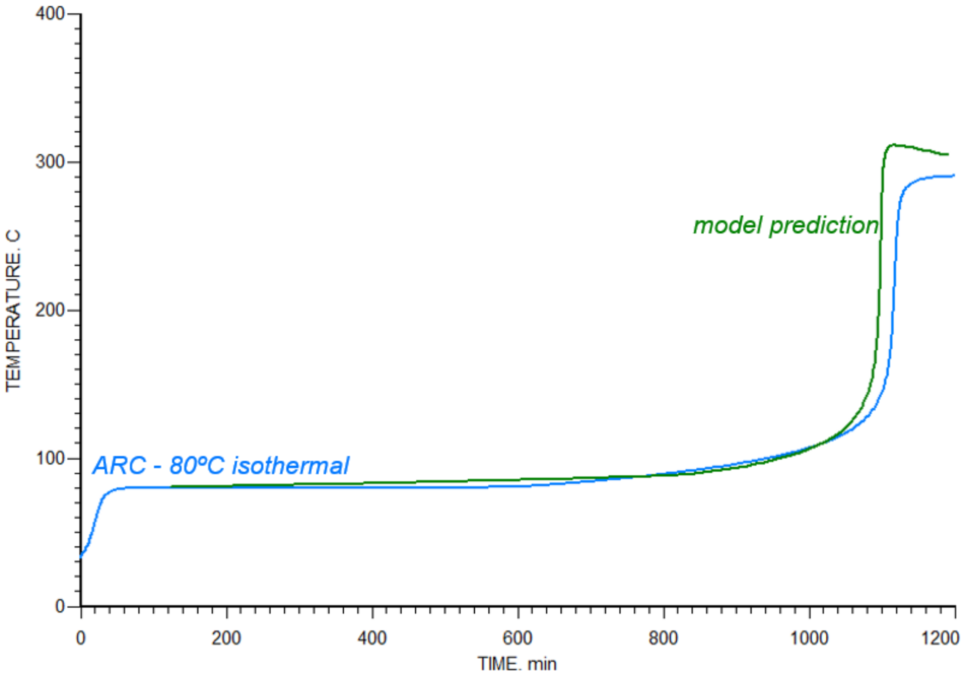

Figure 2: Temperature Profile with Integrated TBC Depletion Model

<u>Detailed Wall Dynamic Simulation</u>

In order to account for detailed equipment wall and fluid heat transfer dynamics, the simulated equipment is segmented into multiple zones, as shown in Figure 4. Detailed heat transfer to/from the surroundings and between the zones are dynamically accounted for. There is no limit on the number of zones a user can specify. The ability to distribute an equipment into multiple segments allows users to closely examine the dynamics of the fluids and equipment wall thermal effects. Other valuable applications of the segmentation approach include the modeling of detailed insulation, external fire, localized or solar heating, and flame jet impingement.

To model the 55-gallon drum, it was assumed that the drum is situated vertically and segmented into five (5) zones. Similar for the railcar, the equipment is divided into five zones, but it is modeled in horizontal orientation.

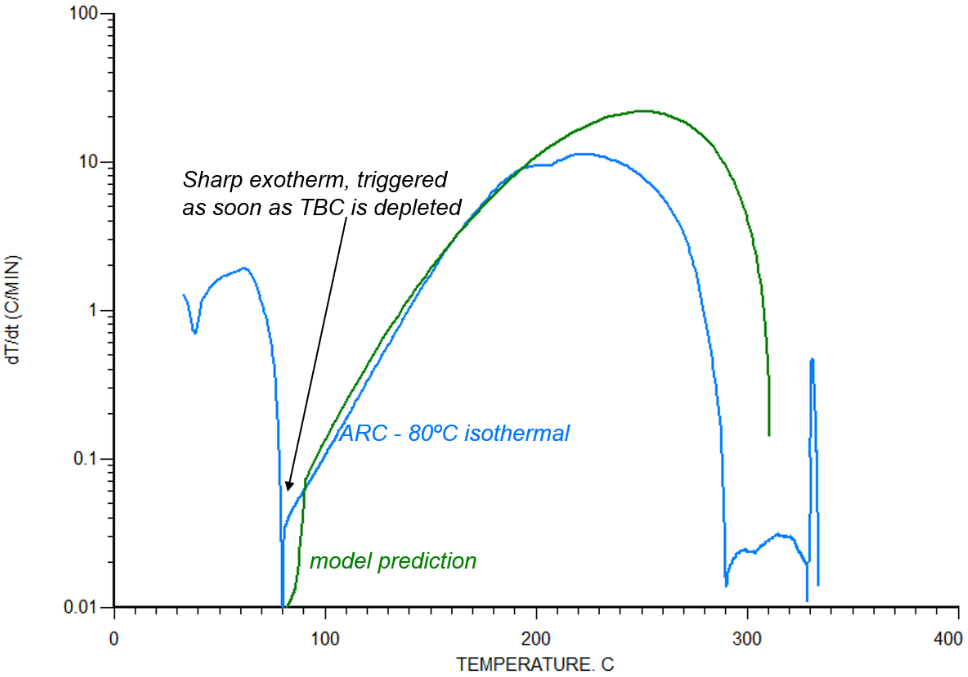

Figure 3: Temperature Rise Profile with Integrated TBC Depletion Model

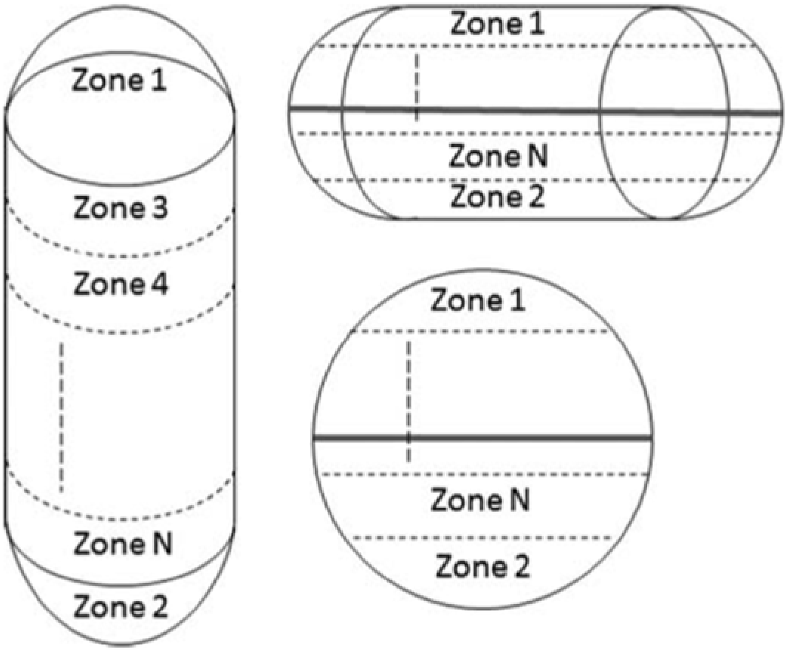

Figure 4. Sample of Equipment Segmentation Scheme

3 Results and Discussions

Analytical Method

Table 4 provides the test summary for the ARC tests and key parameters extracted from the results. The heat-wait-search test reveals an exotherm with onset temperature of 96.8ºC (at exotherm threshold of 0.9ºC/min) and end temperature of 299.5ºC (Figure 5). The maximum temperature rise rate measured was 21.7ºC/min at 246ºC (Figure 6). Note that the cool down pressure measured was 17.6 psia, suggesting that no significant non-condensables generated. The results from the H-W-S test provided good basis for the temperatures selected for isothermal tests.

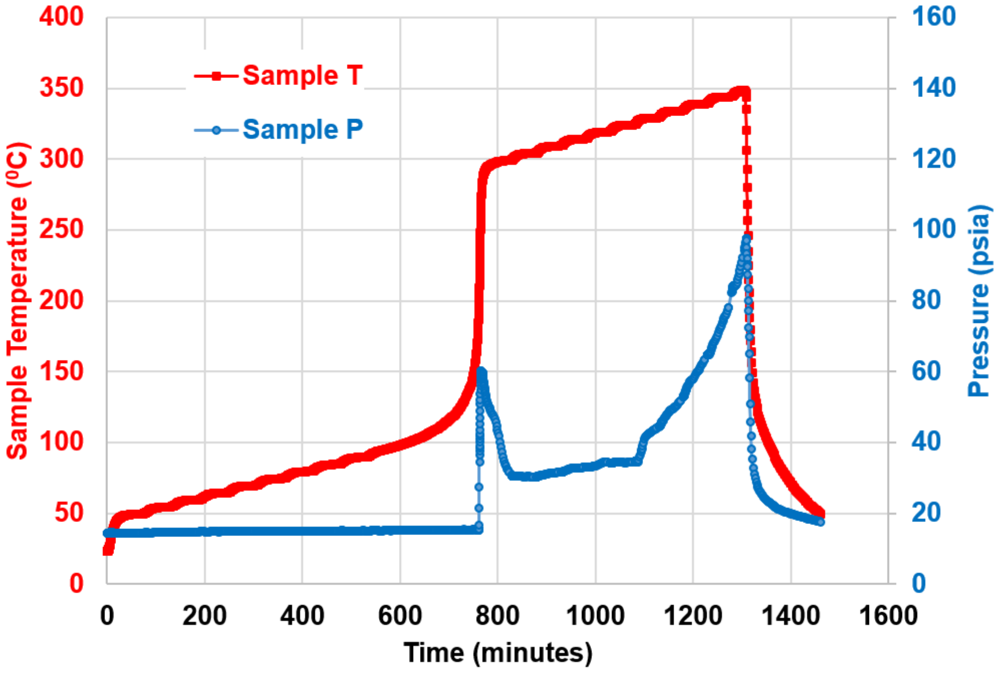

Figure 5: Temperature and Pressure Profiles (H-W-S Mode)

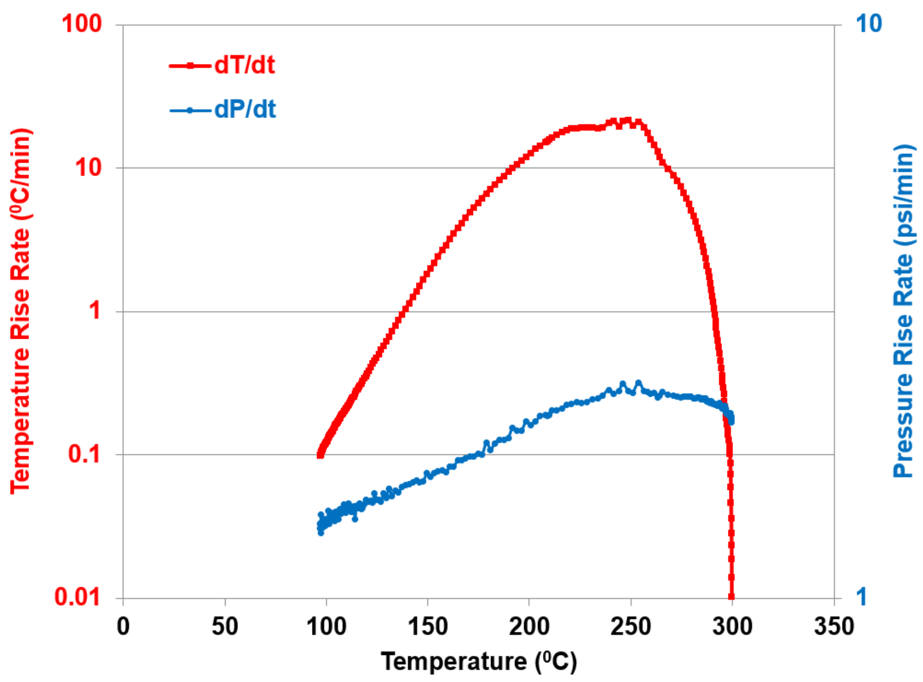

Figure 6: Temperature/Pressure Rise vs Temperature Profiles (H-W-S Mode)

Table 4: Summary of ARC Test results

Key Result Parameter	**H-W-S Mode**	**Isothermal Mode**		
		80^{o}C	***85^{o}C***	***90^{o}C***
Onset temperature, ^{o}C	96.8			
Adiabatic T rise at Phi=1, ^{o}C	288	298	294	298
Heat of reaction, BTU/lb$^{\gamma}$	248	256	253	256
Induction time (min)	N/A	448	224	55
T$_{MR}$ @ phi factor φ=1 (min)	N/A	741	505	337
Activation energy, cal/gmol	18260			

$^{\gamma}$ Specific heat of styrene assumed at 0.477 cal/g/^{o}C

As summarized in Table 4 and illustrated in Figures 7 and 8 for the samples iso-aged at temperature of 80^{o}C, 85^{o}C and 90^{o}C, the induction time measured were 448, 224, and 55 minutes, respectively. The results confirm that the induction time increases exponentially with decrease of sample temperature. A shorter induction time suggests that the inhibitor is depleted faster. In other the words, the higher the temperature, the faster TBC is depleting. The results also show the heat of reactions estimated between 248 and 256 BTU/lb.

Time to maximum heating rates (T_{MR}) were estimated at phi factor equaling to 1 and illustrated in Figure 10. It will be used to estimate the temperature of no return (T_{NR}). The activation energy was estimated from the ARC test data and was found to be 18260 cal/gmol.

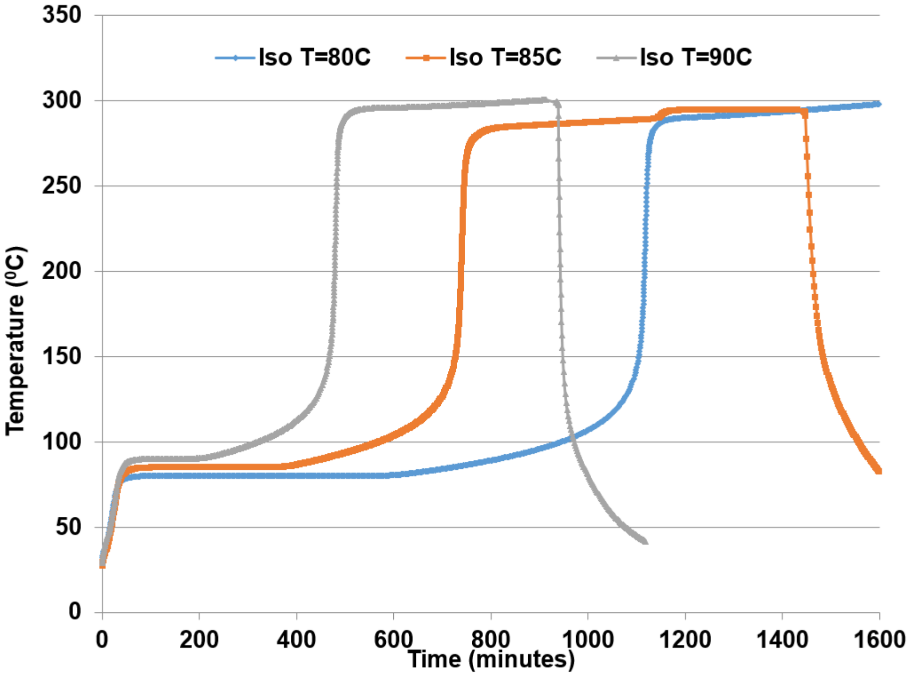

Figure 7: Temperature Profiles for Iso-aging at 80^{o}C, 85^{o}C and 90^{o}C

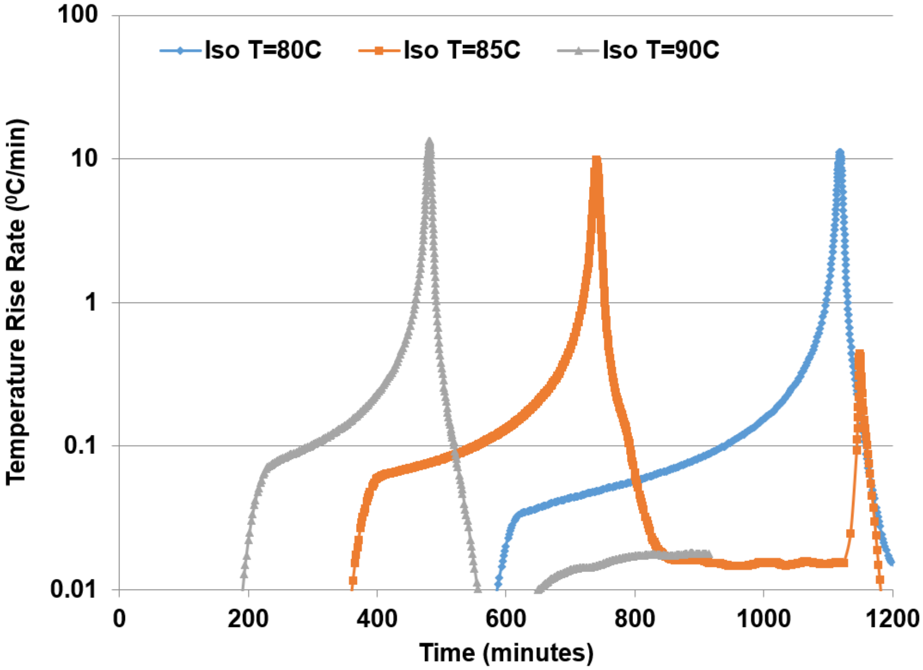

Figure 8: Temperature Rise vs. Time for Iso-aging at 80^{0}C, 85^{0}C and 90^{0}C

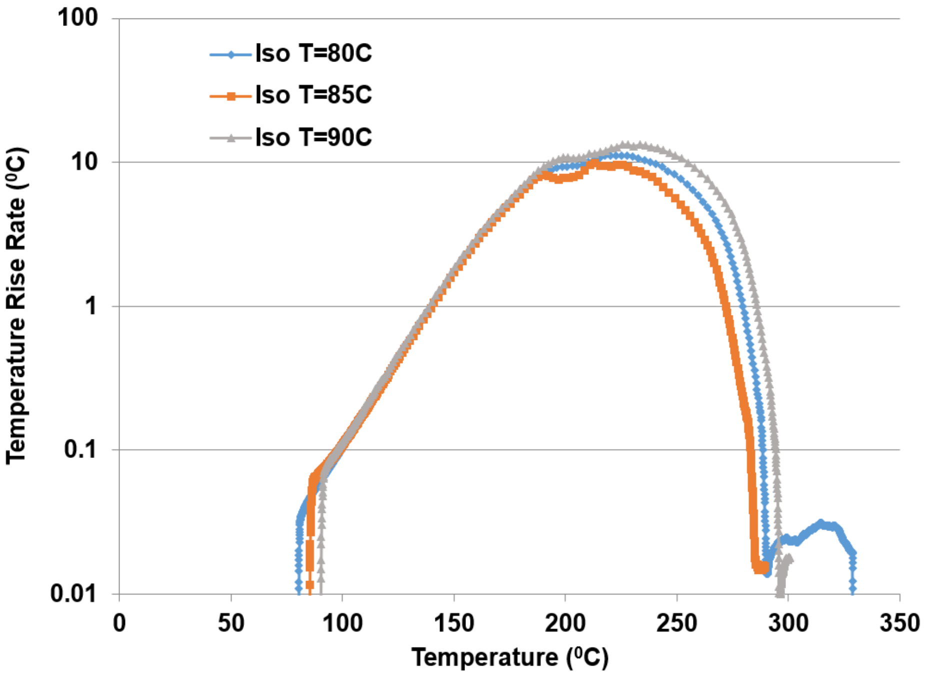

Figure 9: Temperature Rise Rate vs. Temperature for Iso-aging at 80⁰C, 85⁰C and 90⁰C

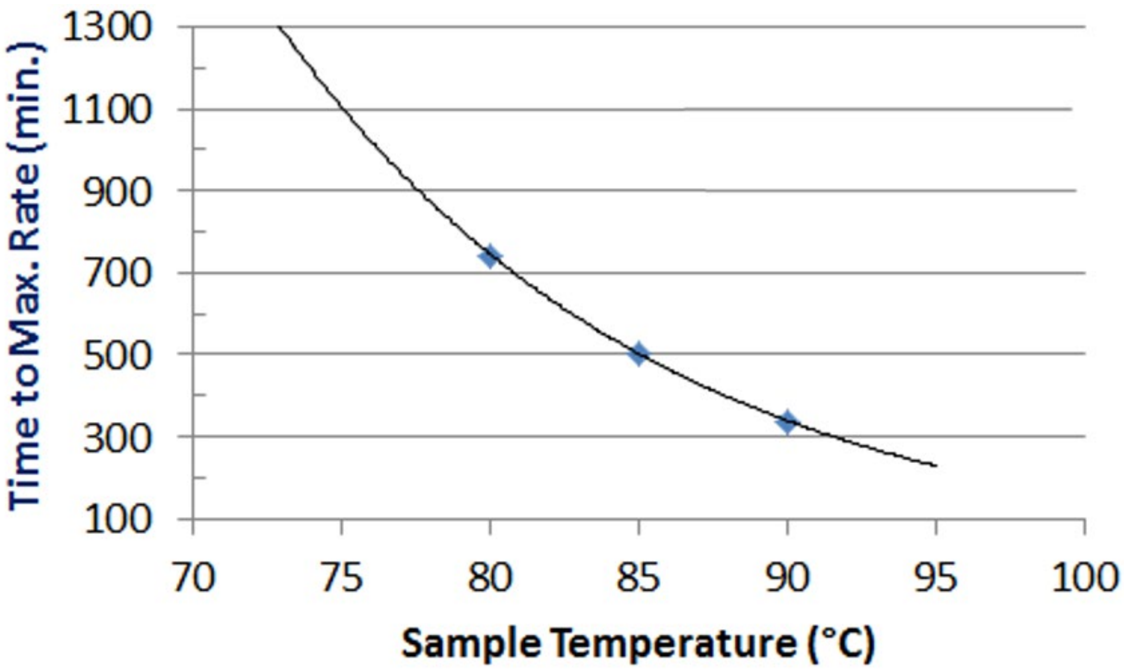

Figure 10: Time to Maximum Rate vs. Temperature Profile

3.2 SADT Determination

Table 4 provides a summary of the key parameters used to estimate the SADT. Note that the 55-gallon drum has a total surface area of 17.31 ft^2, consisting of 413 pounds of styrene. The time constant (τ) was estimated with the use of equation 1, yielding to 5.689h (341.4 min). From Figure 10, the temperature of no return (T_{NR}) was estimated from found to be 89.6°C. Applying equation 2, the SADT of the drum was calculated to be 75.3°C.

Table 5: Estimation of SADT of Styrene for 55-gallon Drum

Parameter	Value
Drum surface area, ft^2	17.31
Styrene density, lb/gal	7.51
Mass of Styrene, lb	413
Heat capacity of Styrene, BTU/lb/°C	0.858
Overall heat transfer coefficient, BTU/h/ft^2/°C	2.00
Activation energy, BTU/gmol	72.50
Constant R, cal/gmol/K	1.987
Time constant (τ), h	5.689
Temperature of no return (T_{NR}), °C	89.6
SADT, °C	75.3

Dynamic Simulation Method

Figure 11 shows the dynamic temperature profiles for the 55-gallon drum. The drum content was assumed starting at normal temperature of 25°C and stored at various ambient temperatures, ranging from 35 to 70°C. The dynamic simulations account for detailed heat transfer among the zones defined and heat exchange to/from the surroundings. At the 35°C storage condition, the results show that the drum content approaches the storage temperature and equalizes with the ambient conditions. Reaching the thermal equilibrium indicates that the any generated heat is effectually dissipated from the drum to the surroundings. The same can be said for the case of the 55°C storage conditions.

As the storage temperature further increases (see 60 to 67°C), the corresponding temperature profiles show that (after 5 days based on 60°C storage condition as example) the drum content temperatures are higher than the storage condition. The fluid temperature higher than the storage condition suggests that the heat generated exceeds the rate dissipated to the surroundings. In all these three cases, the fluid temperature ultimately recedes, indicating reaching a subsequent thermal equilibrium. Full-blown thermal runaway reactions are not expected.

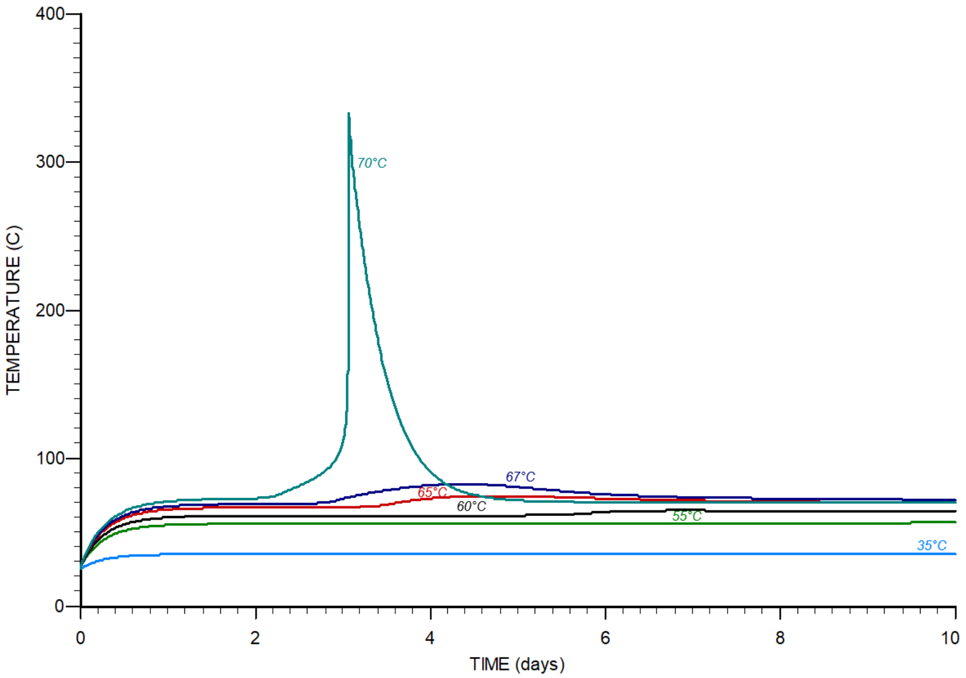

Figure 11: 55-gallon Drum Temperature Profiles at Various Storage Temperatures

At 70°C storage condition, however, the simulations show that the drum would experience a full-blown thermal runaway after three days. The rate of heat generated overpowers the rate dissipated to the surroundings. Figures 12 and 13 shows further details of the drum wall temperatures for the drum stored at 70°C. Notice that initially the fluid temperature is at the lowest. Out of the 5 segments (zones) studied, the top zone has the highest temperature. This is due to a vapor portion (not cooled by the fluid content) and exposed to and heated by the storage ambient condition. After about 1 day (1400 min), the fluid temperature and all zones equalize at 70°C. Figure 13 (magnified) shows that at thermal runaway, the fluid temperature becomes highest (as expected), overcoming the drum metal wall temperatures. Based on the simulations shown, it can thus be concluded that an equivalent SADT for the 55-gallon styrene drum would be 70°C.

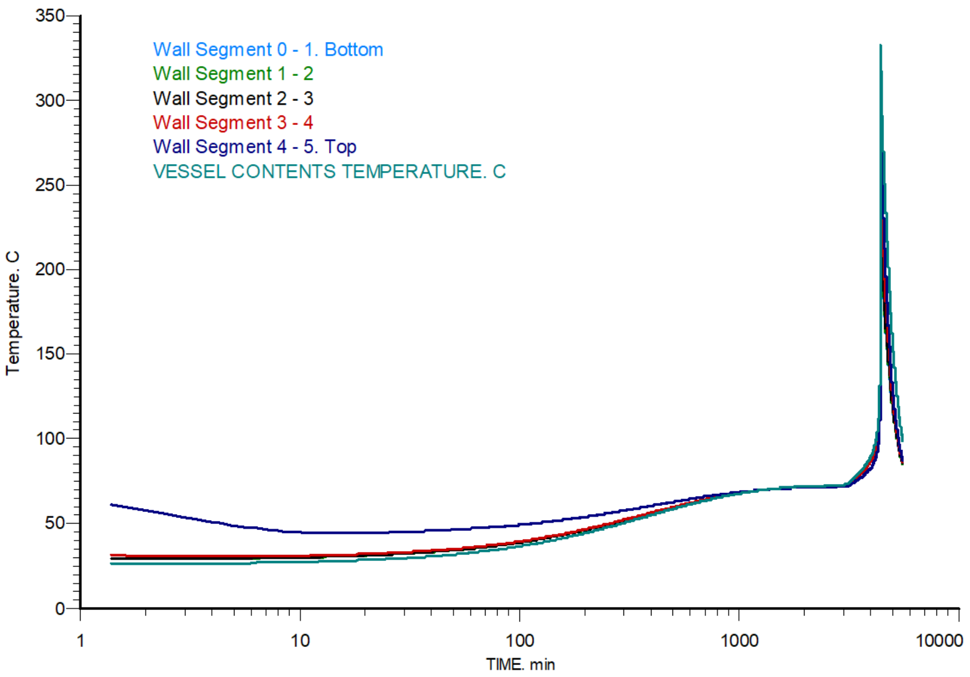

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Figure 12: 55-gallon Drum Stored at 70ºC Shows Thermal Runaway within 7 Days

Figure 14 shows the dynamic temperature profiles for the railcar. Like the drum simulations, the railcar initial content was assumed starting at normal temperature of 25°C. The railcar is stored at various ambient temperatures, ranging from 35 to 70°C. The dynamic simulations account for detailed heat transfer among the zones defined and heat exchange to/from the surroundings. At the 35°C storage condition, the results show that the railcar fluid temperature slowly increases. The fluid temperature higher than the storage condition suggests that the heat generated exceeds the rate dissipated to the surroundings. After 90 days, the railcar's stored content ultimately reaches thermal runaway.

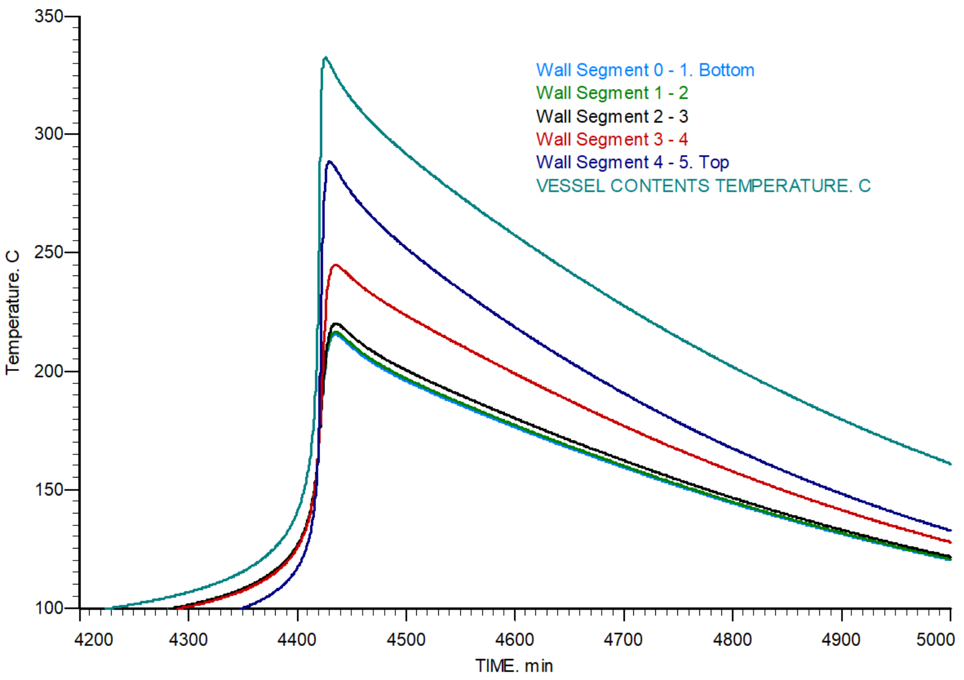

Figure 13: 55-gallon Drum Stored at 70°C (magnified)

As the storage temperature further increases (see 55 to 70°C), the thermal runaway occurs lot faster. The model shows that it would take a little more than 10 days for the railcar content to reach a full-blown thermal runaway when stored at 55°C condition. At 60°C and 65°C, the time to thermal runaway are about 9 and 8 days, respectively. The temperature profile for the 70°C shows that the thermal runaway occurs at about 6.2 days. A more refined simulation shows that the lowest storage temperature that would limit a full-blown thermal runaway within 7 days is 67°C. Based on the simulations shown, it can thus be concluded that an equivalent SADT for the styrene railcar would be 67°C.

Note SADT for a given chemical is depend on the package shapes and sizes. When compared between the 55-gallon drum and railcar, the drum has higher surface area to volume area. Calculations show that difference between the two is a factor of 6.5. In general, a higher surface area to volume ratio has an advantage, providing ample medium to enhance detailed heat transfer mechanisms. As shown in the simulations, the model confirms that the drum can tolerate higher temperature storage conditions.

Figure 15 shows the illustrates the impact when a loss of inhibitor occurs for the railcar stored at 35°C. It could occur as a result of a maintenance/monitoring issue or an incident of inadequate oxygen supply. The simulation shows that railcar can last up to 90 days when maintained properly. In the event of loss of the inhibitor, the railcar would endure less than 22 days. The time difference is almost a factor of 4. What is learned from the kinetic model developed is that it is flexible. One can model the impact of localized heat or effect of insulated equipment. In short, it can simulate any scenarios and for any shapes or sizes of equipment.

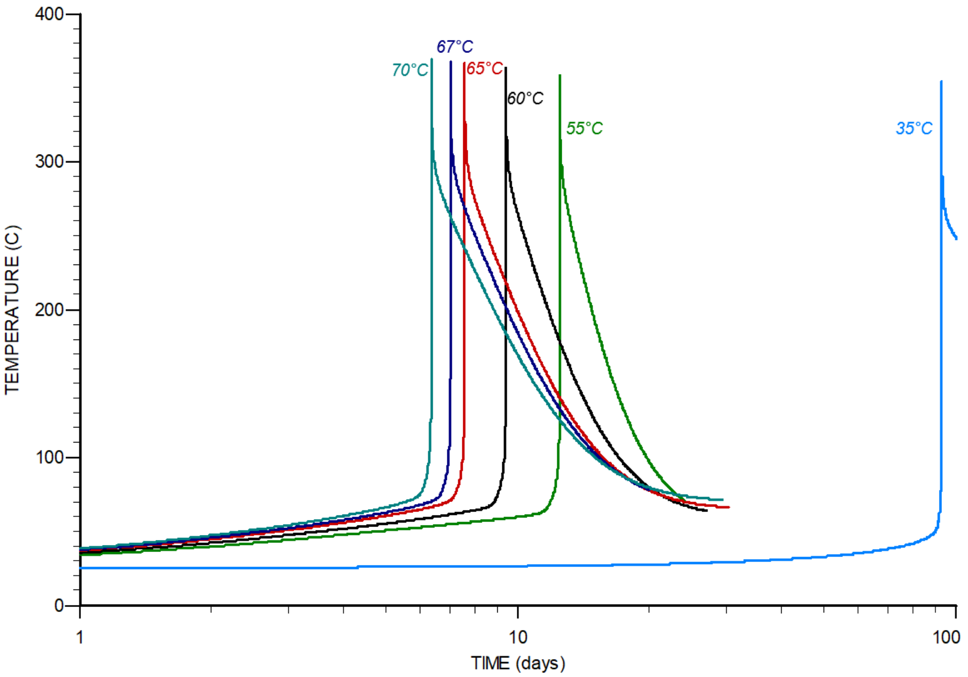

Figure 14: Railcar Temperature Profiles at Various Storage Temperatures

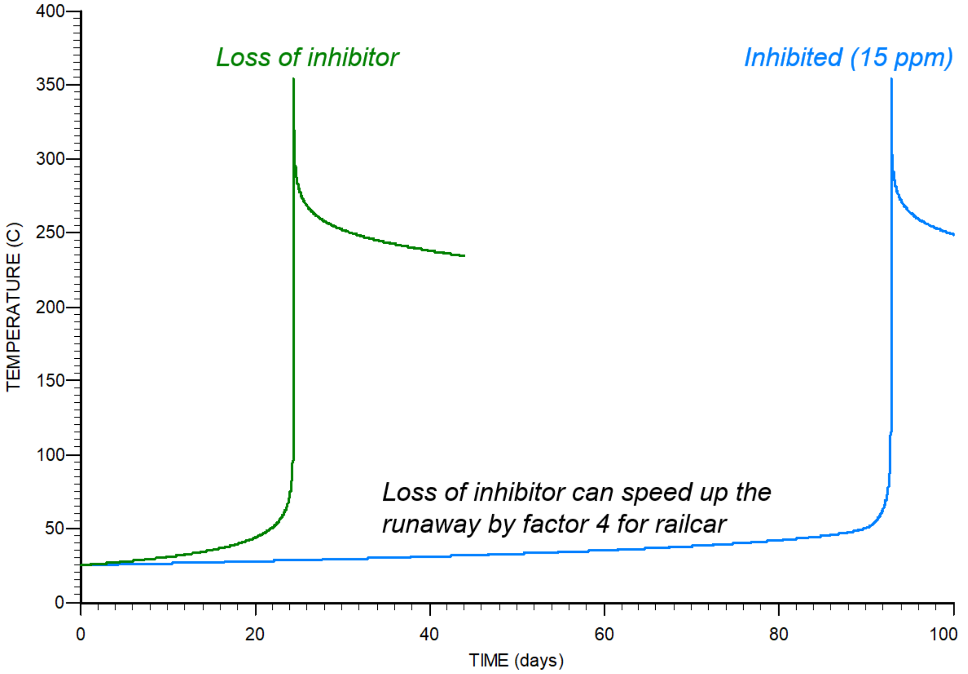

Figure 15. Impact of Loss of Inhibitor in Railcar at 35ºC Ambient Temperature

4 Conclusions

SADT is estimated by fundamental heat balance calculation. It can be calculated analytically or modelled dynamically. Because of a small sample size, the ARC method is cost effective and can serve as a good alternative to the traditionally more expensive methods.

ARC experimental data may be fitted, scaled up, and developed into detailed kinetic models. Given the detailed wall dynamics capability described, the paper demonstrates that the developed models are well equipped to model any shapes and sizes with detailed heat transfer mechanisms considered from and to the surroundings and within the equipment internals.

For the 55-gallon drum the estimated SADT is 75.3°C (analytical method) and 70°C (dynamic simulation method). The dynamic simulation method shows that the railcar would have the SADT of 67°C.

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