WIPP Site Incident Independent Review (WSIIR) Team

09/30/15 Interim Report

(Updated with edits: 10/30/15)

New Mexico Tech
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Contents

Introduction

This document provides an update on the progress of the WIPP Site Incident Independent Review (WSIIR) team. Drum #68660 experienced an exothermic runaway reaction that led to a rupture on February 14, 2014.

Over the last six months our team has reviewed all documentation about the incident including the Accident Investigation Board's reports and additional information on the DOE WIPP Recovery Site, the resources available via the WIPP Waste Information System Public Inquiry web page, the Carlsbad Environmental Monitoring & Research Center (CEMRC) Site WIPP Monitoring website, and the EPA's Review of WIPP Incident website. In addition, the WSIIR team has examined closely the investigation and analyses conducted by both the Los Alamos National Laboratories (LANL) WIPP Incident Investigation Group and the Technical Assessment Team (TAT). WSIIR was briefed by the Los Alamos National Laboratories (LANL) WIPP Incident Investigation Group on July 29, 2015 and the Waste Isolation Pilot Plant (WIPP) Technical Assessment Team (TAT) on August 5, 2015. The key hurdle in the investigation for both teams was that the contents for the drum were not definitively known, and due to heterogeneity, no two drums were identical. Further, due to limited access to drum #68660, physical chemistry analysis was not possible.

In this report we first overview the LANL group's investigation and key findings. We then overview the TAT's investigation by providing a detailed account of our team's questions and the TAT's responses regarding their overall approach, techniques, modeling protocols, and results. Following this overview, we offer our conclusions in each of these areas. Finally, based on the progress of our investigation to date, our team offers our assessment regarding the risk of reopening WIPP.

Overview of LANL Investigation into WIPP Incident

LANL's investigation began in the Spring of 2014. Two teams were tasked with the investigation: one team focused on analyzing the role of the Swheat mixture (referred to elsewhere in this report as organic kitty litter) in the ruptured drum; the other team took a broader focus of the entire incident. These teams reached consistent conclusions throughout their investigation and eventually merged into one team. The charge of this team was as follows:

- to properly understand the February 14, 2014 event
- to render a technical opinion of the event and of the restart of WIPP operations
- to make recommendations on how to avoid a similar event from occurring

Both LANL teams (before they merged) focused their investigation on the chemistry of the event. They considered four areas related to the breach of drum #68660:

1. Changes in waste processing procedures
2. Possible triggers for unstable nitrate salt-fuel mixtures

3. Radiation chemistry
4. Trace metal impurities

Key Findings Presented by LANL

1. The mixture of nitrate salts and organic kitty litter created the potential for an exothermic reaction.
2. A chemical model of a drum with contents similar to drum #68660 confirm the drum should have breached.
3. LANL believes that nitrates + Swheat + water can generate heat which can result into an initial temperature raise of 60° C. This initial temperature is high enough to trigger further exothermic reaction and exponential increase in pressure and temperature.
4. The environmental signature in Panel 7 at WIPP is consistent with the tests on smears from the breached drum, suggesting that the drum #68660 was the only drum that breached.
5. No two drums are the same due to heterogeneity. This could be the reason that one drum breached but not the rest; LANL Cheetah modeling shows that runaway time is highly dependent upon the variables involved.
6. Except for some minor differences, LANL and TAT have similar conclusions regarding the cause of the breach.

LANL does not believe that radiochemistry played a role in the event. A switch from inorganic kitty litter to an organic kitty litter was speculated to have played a large role in the event. It was concluded that the combination of the organic kitty litter with a nitrate salt could create a potential for an exothermic reaction; however; relatively high internal temperatures would be needed to achieve a runaway state. Further studies revealed that mixtures of various nitrate salts with organic kitty litter did not yield an energetic event alone and would require a trigger mechanism to initiate the runaway condition that led to the rupture of the drum. Without knowing the exact contents in drum #68660, recreating the event would prove to be difficult and speculative. Cheetah thermochemical modeling as well as computational fluid dynamic modeling concluded that the result was highly dependent on inputs; without definitively knowing the initial conditions of the drum, modeling was speculative.

In an effort to identify a possible trigger mechanism, LANL focused on the presence of complex metal ions that can participate in nitration reactions of the organic kitty litter. Formations of nitrate esters are a possibility and are exothermic in nature. LANL did not find evidence of nitrate esters. A bismuth-lined glovebox glove was observed in the radiograph of the drum. While LANL could not rule it out entirely, LANL does not believe this glove had a role in the runaway reaction that led to the breach of the drum. Biological organisms were also considered as a trigger for the temperature increase that led to a runaway condition. LANL did not make any definitive conclusions with the exception that biological organisms may have been present if water was present and such biological organisms may have the ability to generate heat.

LANL has been monitoring drums packed similarly to drum #68660 that have not been heated to see if a thermal runaway occurs. Results of these experiments were presented to our team at our July meeting, and at that time no thermal runaway had occurred. It was hypothesized by LANL that oxidation processes in the drums were occurring, but that thermal runaway was not triggered as a result of those processes. If this is indeed the case, then an analysis of the contents of these drums should reveal that the oxidation fuel has been consumed. Further, if an analysis of the contents of the sibling drum, drum #68685, were to show that the oxidation fuel has been similarly consumed, then concerns that other drums containing incompatible chemical mixtures may experience a thermal runaway and breach can be put to rest.

LANL concluded that the mixture of organic kitty litter with nitrate salts (fuel + oxidizer) were combined into the same drum along with a trigger that created a condition in which a runaway thermal event caused the drum to breach. There is uncertainty with regards to the remaining drums that may have a similar chemistry. It is the opinion of the LANL team that a significant heat source, or trigger mechanism would be required for breach. In addition, LANL does not believe that the truck fire played a role in the rupture of the drum.

Overview of TAT Response to WSIIR Team Questions

After closely reading and discussing the TAT's report (published in March 2015), our team generated questions regarding the TAT's overall approach, analytical techniques, modeling and experimental results (our original questions are included in Appendix A. The TAT's written response to our questions are included in Appendix B). During our meeting on August 5, 2015, the TAT explained in greater detail their answers to our questions as well as answered additional questions from our team. This information is summarized in this section along with our team's conclusions.

Methods

The approaches and methods chosen by the TAT were done so in an effort to gain an understanding of the causes of the breach of drum #68660. The TAT relied on a combination of historical records, visual observations (from Project Reach), chemical analysis, small-scale testing, and modeling to aid in answering questions about the breach. The TAT focused on standard forensic chemical analysis as a starting point for understanding the chemistry of drum #68660. Other methods were considered and not used, however; the TAT believes these additional methods would not have added additional insight into the event.

As the TAT charter was to study the breach of the drum 68660 only, they did not conduct modeling or simulation of the sister drum. Drum #68660 was a daughter drum originating from another remediated parent drum. Drum #68685, its sibling drum, coming from the same parent drum, was believed to have significantly different contents than drum #68660. The TAT did not believe that modeling and analysis of the sibling drum (#68685) would provide any insight into the event that caused #68660 to rupture; however our team believes thermal runway modeling of drum #68685 could provide better insight into the modeling protocols; it is our team's opinion that understanding the radiological release event should involve understanding both why drum #68660 ruptured and why other drums containing incompatible chemical mixtures did not rupture.

The TAT interfaced with LANL in an effort to identify potential mixtures that could exhibit exothermic reactivity using small-scale testing methods. These include Differential Scanning Calorimetry (DSC), Automatic Pressure Tracking Adiabatic Calorimetry (APTAC), Thermal Activity Monitor (TAM), and explosive sensitivity tests—friction, electrostatic discharge, impact, and thermal stability. These tests are widely accepted for evaluation of energetic potential of a compound. TAT did not consider modeling ignition of neighboring drums. There is no evidence that any drums other than #68660 breached. While the heat generated from the breach of one drum could cause a neighboring drum to breach, this was not the case.

Our team's overall conclusion regarding TAT's methods: considering the data uncertainty and the restrictions on accessing the breached drum, the approaches used by the TAT are reasonable.

Code

Our team's questions regarding computer codes were addressed. The TAT indicated that they elected to use CTH-TIGER code for equilibrium rather than Cheetah due to the complexity of the reaction makeup. CTH-TIGER is more accurate in complex systems where metals are present. Cheetah is limited in this capability. Sandia National Labs (SNL) used the most recent version of CTH-TIGER (August 30, 2014). The inputs included the proposed reactant mass fractions and the product library. To ensure the code was running properly, SNL used NASA-CEC code as a comparison to ensure values were in agreement. The pressures selected for the CTH-TIGER codes were limited to 1 atm, yet, as our team noted in our questions to TAT, in reality the pressures would be variable. The TAT argued that the possible pressure range in the drum is very narrow and therefore, a model that considers a variable pressure within the drum will not have a prediction much different from what was already achieved. We believe a constant pressure analysis has introduced some approximation in the model prediction but it does not impact the results substantially.

Considering the large number of unknowns and extensive level of uncertainties, our team finds the TAT's selection and use of computer code to be acceptable.

Modeling

With regards to computer modeling, the TAT indicated that it used three models: equilibrium calculations to evaluate equilibrium products at given temperatures, a chemical kinetic model, and a mechanical model. The chemical kinetic model was run to determine gas generation. This kinetic model was "prescriptive" (meaning that it could be adjusted for ignition at a set time—in this case 70 days to mirror the runaway time for actual incident) rather than predictive, as predictive modeling was not achievable without knowing the exact contents of the drum. Further, the chemical kinetic model was not pressure-dependent due to insufficient available data, but the TAT could predict gas generation using the kinetic model. With their prescriptive chemical kinetic setup, the TAT intended to see if runaway at 70 days resulted in reasonable kinetic parameters.

While this modeling attempt offers a valuable approach in understanding the processes involved in the breaching of the drum and we view the TAT's logic for not using a pressure dependent model as reasonable given the uncertainty in input data, our team notes that a downside for the applied model is having too many redundancies such that it can be adjusted for the drum to breach at any time.

In response to our team's questions regarding the predicted heat sources for nitrate salt and neutralized and sorbed liquid in their chemical kinetic model, the TAT clarified that the thermal runaway would have occurred regardless of radioactivity; thus, the cause of the breach is not due to the generated heat by the internal radioactivity of the drum content. As explained by the TAT, ignoring the generated thermal energy by radioactivity can only change the breach time for a relatively short period of time as this source of energy has a small contribution into the overall generated heat. Our team was also assured by the TAT that their heat conductivity assumptions regarding drum #68660's contents were based on measurements of surrogate waste mixtures conducted by Sandia National Laboratories and informed by published literature. Given this clarification, the output of the model in which the body temperature showed almost no increase is acceptable assuming heat conduction was the only mechanism for heat transfer within the drum.

Due to the uncertainties involved regarding the content of the breached drum, a fully coupled model was not used by the TAT, nor was the drum vent part of their models. Our team views the simplified model used by the TAT as reasonable, considering the uncertain parameters involved. Nevertheless, full coupling could have provided more details to explain why the drum breached and account for the role that the vent had in controlling the generated internal pressure. Unfortunately, without access to the breached drum, a comparison of the deformed shape of the physical drum with the output from numerical modeling can't be made. Such a comparison could have provided more information about the rate of internal gas generation and induced pressure. The ongoing physical tests being performed by LANL on the externally heated drums will provide some of this information.

The TAT used an elasto-plastic model to simulate the deformation of the drum. The material constants were obtained from some physical tests, but no simple testing was conducted to verify the behavior of the model; a simple numerical modeling of direct tensile or compressive tests is useful to assure that the prediction of the numerical model is consistent with the expected results before the model is applied for the more complicated situations such as the actual simulation of the drum. The TAT incorporated the hardening behavior of the drum material in their mechanical model. However, the failure was not directly captured; regions which reached the maximum tolerable Mises stress were interpreted as failed regions. These were identified by the contours of Mises stress.

One of our team's questions regarding the mechanical model used by the TAT pertained to the rupturing of the drum. The TAT explained that the model used was an elastic-plastic hardening model that did not explicitly capture the induced ruptures in the body of the drum. The damages or ruptures in the simulated drum were approximately interpreted based on the extensity of the developed strains in the mechanical model used. We view this simplified mechanical model as reasonable considering the uncertainties involved.

The TAT investigated the impact of the February 5, 2014 truck fire on the temperature rise at room 7 of panel 7. They found no evidence of the truck fire triggering the drum breach nine days later. The TAT used a simplified heat source model for the burning of the truck and drew the conclusion that the truck fire had a negligible impact on the temperature change at room 7 of panel 7 where the breached drum was located. This negligible impact suggests that factors other than the truck fire contributed to the breach of the drum. The observations, based on the discussion during our August 5th meeting, indicated that the ventilation was reversed so the heat should have been driven away from the room.

Although the TAT's models are useful in providing insight into the effect the various constituents have on the chemical processes, **our team's overall conclusion is that the models should not be used to predict behavior due to the vast number of parameters and their uncertainties.**

Results

The TAT addressed questions associated with the results provided in their report. Our team noticed that in Table 3-1 of TAT's report there were samples that were not accounted for, and the TAT explained that the reason was because those samples were never collected. While the intention was to obtain five samples, the challenges inherent to sample collection in an extreme environment and time constraints only allowed for three samples to be taken.

Our team questioned the TAT's presentation of drum #68660's ingredients in a figure in their report (Figure 4.2), noting that the layering of the material in drum #68660, as a water-based system would result in reorganization of the layers over time. Their arrangement of these different layers seemed idealistic to our team, but perhaps this model for arrangement of the layers was the only reasonable path forward to establish the initial conditions of the problem. Nevertheless, we think the difference in the material densities of different layers and the existence of pore spaces as mentioned by TAT have encouraged the mixing of the layers during the transportation of the drum causing at least some irregularities along the interfaces between the layers. The TAT acknowledged that it is not possible to determine reactivity at the layer interface. Both the free liquid that is absorbed in the organic kitty litter as well as the nitrate salts mixed with the organic kitty litter can be reactive based on small-scale bench testing. Mixing of the layers could have occurred at any point. If this did occur, the chemical environment could support a localized-runaway reaction. Our team believes the location of initiation matters. For example, if initiation occurs in the vicinity of the drum body, the heat conductivity of the drum body can affect the temperature build up and the rate of gas generation within the drum.

Another question posed by our team concerned the computer model used by the TAT showing localized high temperature after 70 days. We wondered if both heat conduction and convection were considered in the model and if the high temperature gradient observed in the model might be due to unrealistic heat conduction/convection coefficient used. The TAT clarified that the material model parameters were either measured or collected from the literature. The TAT's response helped support that the applied model used was realistic; however, our team believes it would be more realistic if heat convection was allowed within the drum too. We see internal convection as possible due to the gas and bubbles which are generated within the hot environment within the drum. The gas can move around because of the pore spaces within the waste.

Regarding the results achieved by the TAT's investigation of the incident, our team concludes the following:

- **The TAT used generally accepted methods to conduct its investigation.**
- **The conclusions provided by the TAT are reasonable and are consistent with the physical evidence and with other studies.**
- **The TAT's charter was extremely focused. While this narrow focus helps minimize extraneous activity, this approach could lead to overlooking important events that were not considered.**
- **The TAT's conclusion that the organic kitty litter mixed with the nitrate salts untimely resulted in the rupture of drum #68660 is supported by the physical evidence and modeling.**
- **The WSIIR team agrees with the conclusion that radiation in the drum did not play a significant role in the runaway reaction.**

WSIIR Team Assessment of Risk of Reopening WIPP

The TAT analysis, and more conclusively the LANL studies, have determined that the incorporation of organic kitty litter into the processing of waste being prepared for shipment to WIPP ultimately led to the runaway reaction and subsequent rupture of drum #68660. The WSIIR team agrees with this conclusion. Our team further concludes that all the drums containing the organic kitty litter have been accounted for. The drums already in the WIPP repository have been sealed in their respective "panel/rooms". The WSIIR team agrees that the safest way to deal with the drums that have already been placed in the repository is to seal them in place. The WSIIR team concludes that if organic material is removed from the waste stream, the potential for a similar drum rupture will be eliminated. We are concerned with the composition of the remaining drums that contain organic kitty litter. It has been shown that these drums are susceptible to a runaway reaction if exposed to heat. It is imperative that a recovery plan be implemented to return these drums to a stable condition.

Appendix A

Questions for Technical Assessment Team

Following are questions the WIPP Site Incident Independent Review team has compiled after our reading of the TAT report released in late March. They are arranged from general inquiries regarding the overall TAT's approach to specific questions about analytical techniques and modeling and experimental results. At our meeting in June we will look forward to a detailed presentation from the TAT addressing these questions.

Methods

- With what criteria were the methods used by TAT decided upon?
- Were there additional methods considered but not used, and if so, why?
- Did the TAT consider conducting any modeling or simulation on the sibling drum?
- Page 40 refers to the TAT interfacing with LANL : "*as they conducted small scale tests to evaluate potential reactivity within the MINO2 waste.*" What kind of tests were conducted by LANL and what is the MINo2 waste?
- Did the TAT consider modeling a worst case scenario of all sibling drums being in the same room at the same time?

Code

- Why was CTH-TIGER code used instead of Cheetah for modeling?
- What version of the computer code was used?
- What input of the code was used?
- How did the TAT assure the code was running properly?
- <u>Page 28:</u> It appears that the chemical simulation was conducted under a constant pressure of 1 atm. In reality, the pressure was variable. What would be the prediction of the CTH-TIGER code if pressure is considered variable?

Modeling

- Page 29: It appears that two models have been utilized: 1) a chemical model under constant pressure, 2) a mechanical model that has gas pressure as input. Is that the case? Shouldn't the first chemical model be under variable pressure to get more realistic and consistent results?
- Page 31: The finite element model shows that runaway occurs after 70 days, exactly similar to what was observed in reality. Considering many approximations and assumptions in the model, such accurate prediction is very unlikely.
    - Is the accurate prediction due to calibration of the model (e.g. by using heat sources of 0.12 Watt for nitrate salt and 0.17 Watt for neutralized and sorbed liquid layer) to get this very accurate result?
    - Why is the assumed heat conductivity of the contents of drum 68660 so low that in 70 days, almost no increase (only 1° C) in the drum body temperature was realized? This low increase in the temperature of the drum body is not consistent with temperature monitoring of other drums which are being monitored by LANL. Their monitoring shows increase in the body temperature.
- Page 31: It appears that an uncoupled modeling has been used: 1) a chemical model and gas generation. 2) a mechanical model with gas pressure applied inside the drum. Was the drum vent part of the model? Isn't a full coupled model more realistic?
- Page 32: Is the stress analysis of the drum an elasto-plastic or visco-plastic model? What boundary conditions were applied to the drum lid? If the vent was not part of the model, why is it claimed that: "*This slow pressurization was sufficient to overcome the drum vent*"?
- Page 34: The air flow and change in temperature in P7R7 was modeled to find out the impact of the truck fire on Drum 68660. How was the heat source (burning of the truck) modeled in this situation?

- Page 95: "*The hardening curves from the test data were implemented in the analysis for the elastic-plastic model*". How? Did the TAT try to simulate the uniaxial tensile tests? How about the softening? Did the TAT conduct a large deformation analysis?
- Page 97: Second paragraph: Is our reading accurate that the computer program used did not model the drum content? Therefore, is it correct that no gas-drum interaction was modeled? A time varying pressure boundary condition was applied that was not affected by bulging of the drum?
- Page 99-106: The yielding stress (also the stress contours) was either 29×10^3 or 40×10^3 psi. It does not seem hardening was modeled (even though it is claimed to be part of the model). Based on Figs. D10 and D11, steel can carry up to 50×10^3 psi Von-Mises stress, which is not the case in figures reported in pages 99-106.
- Page 107: It is noted that "*the deformation of the lid might provide an indication of the rate of the pressurization*." Have there been any attempts to see the actual deformed shape of the Drum 68660?
- Page 108: "*Without a better understanding of the strain in the closure ring, it was not felt it was advisable to pursue some of these issues. There is uncertainty regarding how consistent the closure ring strain is from drum to drum. An improved understanding of this is advisable prior to pursuing further mechanical modeling with respect to predicting opening pressure*." Can strain gages be installed and used to measure the actual closure ring strain?
- Page 109: It is noted that "*No analyses showed the drum rupture on its sidewall and one would not expect that to happen from this type of a pressurized event*." Was the model used capable of actually showing the rupture in the drum?

Results

- Page 19: Table 3-1 lists the samples collected. Why are samples 4 and 5 not listed or accounted for?
- Based on Fig. 4.2, almost all ingredients of Drum 68660 are lighter than water. Wouldn't this cause the material to mix up? The lighter material should gradually move upward and this especially is encouraged when the drum is shaken and moved, i.e. during its transportation.
- Page 27 (first and second paragraph): "*The chemical and physical forms of these layers and interfaces are different in chemical reactivity and thermal conductivity. The degree of mixing between the layer of neutralized and sorbed liquid and the layer of nitrate-salt admixture is not known".*

  "The physical configuration at the interface of the neutralized-and-sorbed liquid/Swheat Scoop and the nitrate-salt and mixture/Swheat Scoop layers may have formed a localized region of reactivity leading to the thermal-runway event". Based on our previous question about the materials shown in Fig. 4.2 mixing up, how certain are you about the existence of this localized region?
- Page 29: Fig. 4.3: The CTH-TIGER model shows localized high temperature after 70 days. Do you consider both heat conduction and convection in the model? Might the high temperature gradient observed in the model be due to unrealistic heat conduction/convection coefficient used?
- Page 77: 1st paragraph: The X-ray was used to observe the layer interfaces of different materials in Drum 68660. How did the TAT know the arrangement from top to bottom of these materials?
- Page 80: Equation (17) considers the reaction heat sources and heat conduction. How about the convection process?
- Page 94: Are the drum mechanical tests referred to in the literature numerical or physical tests or both?

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Appendix B

Technical Assessment Team Responses to WSIIR Questions

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Waste Isolation Pilot Plant Technical Assessment Team Response to WIPP Site Incident Independent Review Team Questions

July 10, 2015

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7/9/2015
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CONTENTS

LIST OF ACRONYMS AND ABBREVIATIONS

AIB	Accident Investigation Board
APTAC	Automatic Pressure Tracking Adiabatic Calorimetry
atm	atmosphere
DOE	Department of Energy
DSC	differential scanning calorimetry
EM	[Office of] Environmental Management
ESD	electrostatic discharge
GC	gas chromatography
IC	ion chromatography
ICP	inductively coupled plasma
INL	Idaho National Laboratory
LANL	Los Alamos National Laboratory
LC	liquid chromatography
LLNL	Lawrence Livermore National Laboratory
MS	mass spectrometry
NASA	National Aeronautics and Space Administration
NMT	New Mexico Tech
OES	Optical emission spectrometry
ORNL	Oak Ridge National Laboratory
P7R7	Panel 7 Room 7
PNNL	Pacific Northwest National Laboratory
Pu	plutonium
R&D	research and development
SEM-EDS	scanning electron microscopy-energy dispersive x-ray fluorescence spectroscopy
SITI	Sandia Instrumented Thermal Ignition
SNL	Sandia National Laboratories
SRNL	Savannah River National Laboratory
TAM	Thermal Activity Monitor
TAT	Technical Assessment Team
TEA	triethanolamine
TG-MS	thermogravimetric- mass spectroscopy analysis
WIPP	Waste Isolation Pilot Plant
WSIIR	WIPP Site Incident Investigation Review
XRD	x-ray diffraction [spectroscopy]
XRF	x-ray fluorescence

1.0 INTRODUCTION

PURPOSE

This document provides the responses of the Waste Isolation Pilot Plant (WIPP) Technical Assessment Team (TAT) to questions asked by the WIPP Site Incident Independent Review (WSIIR) team about the WIPP TAT report released in March 2015. The WIPP TAT responses address both the general inquiries regarding the TAT's overall approach and the specific questions about analytical techniques and modeling and experimental results. The responses are arranged in the same order as the questions received. At the request of the WSIIR team, WIPP TAT representatives will participate in the WSIIR team's meeting scheduled for August to discuss the WIPP TAT responses.

BACKGROUND

WIPP Radioactive Material Release Event

On February 14, 2014, an incident in the WIPP underground repository resulted in the release of radioactive material into the environment. No personnel were determined to have received external contamination; however, twenty-one individuals were identified through bioassay to have low-level amounts of internal contamination, and trace amounts of radioactive material were detected off-site following the incident. [AIB, April 2014]

WIPP Accident Investigation Board

The Department of Energy (DOE) Office of Environmental Management (EM) expanded the scope of the Accident Investigation Board (AIB) that had been established to investigate the February 5, 2014 salt-hauling truck fire in the WIPP underground to include investigation of the WIPP radiological release. The scope of the AIB's investigation is broad and includes identifying all relevant facts; determining direct, contributing, and root causes; developing conclusions; and determining measures to prevent recurrence. [Moury, March 2014]

The AIB's Phase 1 Investigation Report released in April 2014 concludes that the direct cause of the event was the "breach of at least one transuranic (TRU) waste container in the underground which resulted in airborne radioactivity escaping to the environment downstream of the HEPA filters." The Phase 1 Investigation Report notes that "the exact mechanism of container failure . . . is unknown at this time and must be determined once access to the underground is restored. This will be investigated in Phase 2." [AIB, April 2014]

WIPP Technical Assessment Team

To complement the AIB investigation, DOE established the WIPP TAT to determine to the extent feasible the particular mechanism(s) and chemical reactions that may have resulted in the failure of the waste drum and release of material in WIPP. This narrowly defined scope allowed the TAT to confine its investigation to the technical aspects of the release while the AIB conducted its broader investigation.

The TAT was chaired by the Savannah River National Laboratory (SRNL) and composed of members from SRNL and Lawrence Livermore National Laboratory (LLNL), Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNNL), and Sandia National Laboratories (SNL). The TAT's national-laboratory team approach provided scientific and technical rigor and credibility needed to assess the event and support DOE's implementation of a WIPP recovery plan.

The TAT undertook an extensive process of historical data review, sample collection and analysis, laboratory testing, and computational modeling to understand the release event in WIPP. Investigative constraints, such as incomplete documentation of the processes used to create the drum that breached and the physical inaccessibility of the breached drum in WIPP, created uncertainties, which made collection and interpretation of scientific data alone insufficient to reconstruct the event fully. However, the TAT evaluated the uncertainties and utilized expert assessments of available information and analytical data to fulfill its charter.

Using this strategy, the TAT reached its overarching conclusion and five associated key judgments. (*Waste Isolation Pilot Plant Technical Assessment Team Report*. March 17, 2015. Savannah River National Laboratory. SRNL-RP-2014-01198. http://energy.gov/em/downloads/technical-assessment-team-report)

WIPP Site Incident Independent Review (WSIIR) Team

The WSIIR is an independent review team established by the State of New Mexico to review the events leading up to the closure of WIPP and recommend changes needed to resume operations.

The WSIIR team is composed of faculty, administrators, and staff of New Mexico Tech (NMT) and is led by NMT's Vice President for Research and Economic Development.

In addition to examining the circumstances that led to the rupture of the waste containment drum in WIPP and defining the magnitude of the reaction, the WSIIR will conduct open-to-the-public meetings in the Carlsbad area to collect and understand public concerns regarding WIPP operations. The information gained from these meetings will aid the team in developing recommendations for future operations.

The expected result of this work will be a more resilient, safe, and robust program that will restore credibility with and support from the community and state.

As part of their mission to conduct a transparent review, all WSIIR work is documented and available to the public. Beginning in August 2015, the WSIIR team will publish quarterly reports accessible to the public. (http://www2.nmt.edu/wsiir)

2.0 WIPP TAT RESPONSES TO WSIIR TEAM QUESTIONS

2.1 METHODS

1. With what criteria were the methods used by TAT decided upon?

   Approaches and methods used by the WIPP TAT were selected to answer questions that were central to gaining an understanding of the underlying cause(s) of the breach of LANL Drum 68660. The WIPP TAT relied on historical records, visual observations, chemical analyses, small-scale testing, and modeling to characterize the release event and answer questions about the nature and causes of the release. This strategy was dictated in part because the site of the release was inaccessible, precluding direct examination and collection of samples for analysis. The TAT used accepted principles of forensic science, analytical and radioanalytical chemistry, and thermochemical and mechanical modeling as well as tractability, quality control and assurance, and peer review to guide the selection and use of methods of inquiry. Proposed methods were discussed, vetted and approved by the WIPP TAT prior to implementation.

2. Were there additional methods considered but not used, and if so, why?

   Yes, additional methods were considered for application to sample analysis, modeling, material characterization, and sub-scale drum testing, but not used. In some cases this was because methods changed based on sample condition and availability or evolving TAT understanding of WIPP conditions and waste characteristics. In general, methods that were considered but not used may have refined elements of the TAT's understanding of the event but were not expected to substantially affect its conclusions.

3. Did the TAT consider conducting any modeling or simulation on the sibling drum?

   No, modeling of drums other than 68660 was not considered. Modeling of a thermal runaway was conducted for Drum 68660 because it was the drum known to have breached at the time of the TAT study. The contents of sibling Drum 68685 (solid waste and a lead liner) are significantly different from the contents of Drum 68660 (which received the job waste and absorbed liquids). Thermal runaway modeling of Drum 68685 would not provide direct insight into the behavior of Drum 68660.

4. Page 40 refers to the TAT interfacing with LANL : "as they conducted small scale tests to evaluate potential reactivity within the MINO2 waste." What kind of tests were conducted by LANL and what is the MINo2 [sic] waste?

   The MIN02 is a waste stream generated by LANL in the 1970s and 1980s from the recovery and purification of Pu. Details are in Section 3.1 (p.17) and Appendix E (p. 150) of the WIPP TAT report. The process resulted in material consisting primarily of metal nitrate and oxalate salts. It is from this waste stream that the parent of Drum 68660, Drum S855793, was generated. Given knowledge of the MIN02 waste stream and the remediation processes that generated Drum 68660, assessments of potential mixtures within Drum 68660 could be determined for characterization of exothermic reactivity using small-scale testing. After the breached drum was established to contain MIN02 waste, LANL performed a number of bench-scale tests to evaluate the reactivity of mixtures of the components of the MIN02 waste stream, neutralizing agents and the Swheat Scoop®. These results were reported periodically to the TAT through presentations, reports, and teleconferences. LANL's testing included a wide range of surrogate waste mixtures using Differential Scanning Calorimetry (DSC), Automatic Pressure Tracking Adiabatic Calorimetry (APTAC), Thermal Activity Monitor (TAM), and explosive sensitivity tests (Impact, ESD, Friction, DSC, and Vacuum Stability). These findings, along with MIN02 waste stream characterization data, provided input to the deliberations of the TAT, which included independent bench-scale reactivity testing at SNL and PNNL. A summary report of the LANL reactivity testing is provided in the report authored by D.L. Clark and D.J. Funk, "Chemical

Reactivity and Recommended Remediation Strategy for Los Alamos Remediated Nitrate Salt (RNS) Wastes", LA-UR-15-22393, Feb. 17, 2015; cited in the TAT report as LA-CP-15-20082.

5. Did the TAT consider modeling a worst case scenario of all sibling drums being in the same room at the same time?

   No. Co-location or proximity of sibling drums is not believed to significantly affect the likelihood of ignition. However, an assessment of the effect of an igniting drum on a neighbor drum was made and is discussed in the "External heating" section (p. 81) of the report. Although this assessment showed that ignition of a drum due to external heating following ignition of another drum is possible, no evidence of additional drums breaching or having extensive discoloration was found.

2.2 CODE

6. Why was CTH-TIGER code used instead of Cheetah for modeling?

   Any equilibrium code would have been appropriate for the calculations conducted as long as an appropriate library of potential products was utilized. CTH-TIGER was chosen for this effort specifically as it has been shown to be more accurate when calculating equilibrium properties for reactants composed of a large number of atoms including metals. (Hobbs ML, Brundage AL, and Yarrington CD, "JCZS2i: An Improved JCZ Database for EOS Calculations at High Temperature and Pressure" 15th Int. Det. Symp, San Francisco, CA (2014))

7. What version of the computer code was used?

   CTH-TIGER is maintained by SNL. The most recent version of CTH-TIGER was used and committed to the SNL version control repository on August 30, 2014.

8. What input of the code was used?

   The input to CTH-TIGER included the reactant mass fractions and the product library. A good reference for the Jacob, Cowperthwaite, Zwisler, Sandia (JCZS) product library used is provided in Hobbs, ML, Baer MR., McGee BC, "JCZS: An Intermolecular Potential Database for Performing Accurate Detonation and Expansion Calculations," Propellants, Explosives, Pyrotechnics, 24, 269 (1999). This library uses the same product species found in the Joint Army, Navy, NASA, Air Force (JANNAF) tables found in Chase MW, Davies CA, Downey JR, Frurip DJ, McDonald RA, Syverud AN, JANNAF Thermochemical Tables, Third Edition, Journal of Physical and Chemical Reference Data, 14 (1985).

9. How did the TAT assure the code was running properly?

   The code has been extensively compared to detonation properties as well as to the NASA-CEC code for rarefied gas dynamics as shown in the paper by Hobbs et al. (2014), cited above, to validate its results. The code has also been used to reproduce the water phase diagram, water hugoniot, sound speed data, etc. It is recognized that the equation-of-state used in an equilibrium code impacts the results. Specific to this work, a check was conducted on the CTH-TIGER results. As a check, selected equilibrium points with both the NASA-CEC and the CTH-TIGER codes were conducted and demonstrated to provide similar results.

10. Page 28: It appears that the chemical simulation was conducted under a constant pressure of 1 atm. In reality, the pressure was variable. What would be the prediction of the CTH-TIGER code if pressure is considered variable?

    In comparison to the calculations shown on page 28 which found the adiabatic flame temperature to be 618 °C at 1 atm, at 2 atm the adiabatic flame temperature is predicted to be 642°C. The pressure is believed to be limited to this range by a combination of the drum vent and the failure pressure of the drum lid closure.

2.3 MODELING

11. Page 29: It appears that two models have been utilized: 1) a chemical model under constant pressure, 2) a mechanical model that has gas pressure as input. Is that the case? Shouldn't the first chemical model be under variable pressure to get more realistic and consistent results?

    There were three models used: 1) equilibrium calculations to determine the equilibrium products at given temperatures (CTH-TIGER), 2) a chemical kinetic model with three representative processes and associated kinetics, and 3) a mechanical model for the drum response to pressure. The chemical kinetic model was a "prescriptive model" as opposed to a "predictive model", in that it used kinetics intentionally adjusted to result in ignition in 70 days. Insufficient data were available to develop a pressure-dependent kinetics model, so the kinetics for this model were not pressure-dependent and therefore provided the same answer whether or not the gases were vented or remained sealed within the vessel. However, because the degree of reaction relates the heat released to the amount of gas generated, the kinetic model also predicts gas generation. The amount of gas formed can be converted to pressure depending on the assumed degree of confinement. This rate was used as a limiting condition for the drum mechanical model. After ignition, the dynamic burn and subsequent rapid pressurization were not calculated.

12. Page 31: The finite element model shows that runaway occurs after 70 days, exactly similar to what was observed in reality. Considering many approximations and assumptions in the model, such accurate prediction is very unlikely.

    It is important to keep in mind that the model was prescribed to undergo thermal runaway at the time it did by adjustment of the activation energies used in the model. This was done to demonstrate the feasibility of the mechanism and to provide a tool for associated analyses. The detailed information required to develop a predictive model (i.e., identification of rate-determining processes and associated kinetics) does not exist and cannot be determined with any certainty given limitations in knowledge regarding the drum contents and their distribution. Therefore, the model is prescriptive rather than predictive. The kinetics used were adjusted to match the apparent 70-day ignition time but could be adjusted for ignition at any time. The main objective of this exercise was to determine if thermal runaway was an ignition mechanism, and the result was that the model was able to replicate ignition at 70 days with realistic kinetic parameters. In addition, the model provided a tool to conduct related analyses, e.g., estimation of the wall temperature at ignition, sensitivity to input parameters and boundary conditions, and sensitivity to external heating.

13. Is the accurate prediction due to calibration of the model (e.g. by using heat sources of 0.12 Watt for nitrate salt and 0.17 Watt for neutralized and sorbed liquid layer) to get this very accurate result?

    The kinetics in the thermal chemical model were prescribed as described previously. The constant heat sources are real numbers determined from the amount of radioactive decay in each layer. See Appendix E, Table E-9 (p. 160) of the WIPP TAT report. This is a very small source of energy. If we turned off this source, the ignition would have been delayed by about 5 days using the same kinetics. The point is that it was not because of the presence of radioactivity that the runaway occurred, which was an important question for the TAT. The thermal runaway would have occurred regardless of the radioactivity. More details of this assessment are discussed in Appendix D (page 82) of the WIPP TAT report.

14. Why is the assumed heat conductivity of the contents of Drum 68660 so low that in 70 days, almost no increase (only 1° C) in the drum body temperature was realized? This low increase in the temperature of the drum body is not consistent with temperature monitoring of other drums which are being monitored by LANL. Their monitoring shows increase in the body temperature.

    The thermal conductivity of surrogate waste mixtures was measured at SNL in the SITI apparatus using the methodologies discussed in Erikson WW, Cooper MA, Hobbs ML, Kaneshige MJ, Oliver MS, Snedigar S., "Determination of thermal diffusivity, conductivity, and energy release from the internal temperature profiles of energetic materials," International Journal of Heat and Mass Transfer, 79, 676 (2014) and was typical for non-metallic granular solids. Previous work has shown that the surface temperature of drum-scale thermally decomposing objects remains very close to ambient temperature up to ignition. We have not seen any temperature measurements on drums being monitored by LANL that indicate internal heating and would not expect such indications given how the measurements have been made, namely on the outside of waste boxes containing waste drums and empty drums.

15. Page 31: It appears that an uncoupled modeling has been used: 1) a chemical model and gas generation. 2) a mechanical model with gas pressure applied inside the drum. Was the drum vent part of the model? Isn't a full coupled model more realistic?

    The thermochemical model calculated the temperature profile within the drum over the 70 days leading to ignition. The mechanics model simulated the mechanical response of the drum after ignition, when significant pressurization occurred. Because the two models were used over different times and time scales, direct coupling was not attempted. Since coupling of the models would be primarily through pressure loading resulting from gas generation, as modified by losses through the drum vent, the vent was not part of either model.

    While a fully coupled model would have the potential to be more accurate and address certain scenarios such as a blocked vent, this was not necessary to meet the objectives of the TAT and would require significantly more information than was available.

16. Page 32: Is the stress analysis of the drum an elasto-plastic or visco-plastic model? What boundary conditions were applied to the drum lid? If the vent was not part of the model, why is it claimed that: "This slow pressurization was sufficient to overcome the drum vent"?

    The stress analysis of the drum used an elastic-plastic model.

    The boundary conditions applied to the drum lid were a) the material contact between the closure ring, the drum body, and the lid and b) the applied pressure condition. In addition, c) for some cases a pressure load consistent with the weight of the MgO was applied, and d) some cases were analyzed with a surrogate drum on top of the pressurized drum.

    The vent was not part of the mechanical model of the drum.

    It is claimed "This slow pressurization was sufficient to overcome the drum vent" because even the slower pressurization rate simulated in these mechanical analyses simulates a pressure generation event (ignition) that is fast enough to overcome any reduction due to a working vent. Two different pressurization rates were modeled to demonstrate what such an event might do to the drum. These were not specific to a certain event, but are considered within a regime of potential runaway type events.

17. Page 34: The air flow and change in temperature in P7R7 was modeled to find out the impact of the truck fire on Drum 68660. How was the heat source (burning of the truck) modeled in this situation?

A detailed model of the combustion was not used or deemed necessary. Rather, fires with constant thermal outputs of 5 or 10 MW deposited energy into the flows that were estimated for the mine air shafts. As indicated in the footnote on page 128, the 5 and 10 MW numbers were incorporated from AIB analyses. Flow conditions and other important factors at the time of the fire are poorly known. Inputs for more detailed models of the combustion cannot be specified with confidence. Consequently, as described in Appendix D, the analyses of the fire products flowing toward the distant P7R7 were handled parametrically both in terms of the fire's thermal output and the flow conditions. These analyses indicated only small temperature rises at P7R7.

More detailed analyses cannot be supported with reliable descriptions of required detailed boundary conditions, and these simpler energy balances consistent with first laws indicate that the fire's output could not reach the waste array. This conclusion was true even with conservative assumptions regarding the fire's energy deposition into the shaft air in the immediate vicinity of the truck.

18. Page 95: "The hardening curves from the test data were implemented in the analysis for the elastic-plastic model". How? Did the TAT try to simulate the uniaxial tensile tests? How about the softening? Did the TAT conduct a large deformation analysis?

The Sierra/Solid Mechanics model designated as "elastic_plastic" was used for the analyses that used the "original mechanical property estimate" (based on Ludwigsen, J. S., D. J. Ammerman, and H. D. Radloff. "Analysis in Support of Residues in the Pipe Overpack Container. 1998. SAND98-1003. Sandia National Laboratories. Albuquerque, NM). This model is an elastic-plastic, linear-hardening model. Linear hardening generally refers to the shape of a uniaxial stress-strain curve where the stress increases linearly with the plastic, or permanent, strain. The model used was the isotropic version.

The Sierra/Solid Mechanics model designated as "ml_ep_fail" was used for the analyses that were based on the mechanical tests from the sample drum lid and closure ring. This model is the multi-linear, elastic-plastic hardening model with failure. However, failure was not implemented. It is similar to a power-law hardening model (common in most finite element analysis codes) except that the hardening behavior is described with a piecewise-linear curve as opposed to a power law. For these analyses, the piecewise-linear curves were based on actual tensile tests performed on coupons from the sample lid and closure ring.

We did not simulate the uniaxial tensile tests. Mechanical properties are derived from the tests, and simulation of the tests is not necessary.

Softening was not included in the analysis.

The Sierra/Solid Mechanics analyses presented are all large deformation analyses.

19. Page 97: Second paragraph: Is our reading accurate that the computer program used did not model the drum content? Therefore, is it correct that no gas-drum interaction was modeled? A time varying pressure boundary condition was applied that was not affected by bulging of the drum?

It is correct that no "gas-drum" interaction was modeled. The pressure on the surface of the drum varied only as a function of time. The magnitude of the pressure did not vary as a function of the internal volume of the drum. The pressure was applied normal to the surfaces of application. So, as the surfaces deformed, the pressure direction remained normal to the surface.

20. Page 99-106: The yielding stress (also the stress contours) was either 29×103 or 40×103 psi. It does not seem hardening was modeled (even though it is claimed to be part of the model). Based on Figs. D10 and D11, steel can carry up to 50×103 psi Von-Mises stress, which is not the case in figures reported in pages 99-106.

    Hardening was modeled. The figures on pages 99-106 are plotted with a maximum contour limited to the yield value. So, anywhere in the figure that the color is fully red means that the Von-Mises stress is at the yield value or greater. The purpose of plotting the figures this way was to demonstrate as simply as possible the regions that are at or above yield.

21. Page 107: It is noted that “the deformation of the lid might provide an indication of the rate of the pressurization.” Have there been any attempts to see the actual deformed shape of the Drum 68660?

    Due to radiation hazards to personnel, no visual inspections of the room or breached drum were allowed other than the images obtained remotely by the Accident Investigation Board in May and then later in Project Reach. The TAT used the photographs available from these two exercises. However, it was difficult to see the actual shape of the lid because it was covered with MgO.

22. Page 108: “Without a better understanding of the strain in the closure ring, it was not felt it was advisable to pursue some of these issues. There is uncertainty regarding how consistent the closure ring strain is from drum to drum. An improved understanding of this is advisable prior to pursuing further mechanical modeling with respect to predicting opening pressure.” Can strain gages be installed and used to measure the actual closure ring strain?

    Yes, strain gages could be installed and used to get some indication of the actual closure ring strain. However, there would still be some uncertainty with respect to how that related to Drum 68660. It would remain uncertain how the properties of any tested “sample” drum material might relate to drums that have already been put into service.

23. Page 109: It is noted that “No analyses showed the drum rupture on its sidewall and one would not expect that to happen from this type of a pressurized event.” Was the model used capable of actually showing the rupture in the drum?

    No specific method was applied to the analyses to predict “rupture” of the metals. However, rupture in this material would most likely be preceded by very high strains concentrating locally. The model is capable of predicting such concentration of strains.

2.4 RESULTS

24. Page 19: Table 3-1 lists the samples collected. Why are samples 4 and 5 not listed or accounted for?

    Samples 4 and 5 were not collected. We were prepared to collect up to five samples from the surface of the drum stack at 15-5 and the lip of 16-4 in P7R7 if the constraints of the August 15, 2014 sampling operation allowed; we collected three samples from those locations during that operation. The chain-of-custody document received by the TAT lists those three samples (Samples 1, 2, and 3) from 15-5 and 16-4 as well as two samples of MgO (Samples 6 and 7). All were accounted for by the TAT. A copy of the chain-of-custody is available in *Sampling Report for August 15, 2014 WIPP Samples*, December 19, 2014, Forensic Science Center, Lawrence Livermore National Laboratory, LLNL-TR-667000.

25. Based on Fig. 4.2, almost all ingredients of Drum 68660 are lighter than water. Wouldn't this cause the material to mix up? The lighter material should gradually move upward and this especially is encouraged when the drum is shaken and moved, i.e. during its transportation.

    The densities listed in Figure 4-2 are the overall bulk density of each layer and not of the specific density of the material in the mixture. The bulk density includes any void volume that may have existed in each layer, which would decrease the bulk density with increasing void fraction. That being said, the TAT did not conduct experiments to evaluate the post-mixing and separation of materials, and associated kinetics, within the mixtures of each layer and amongst the individual layers that may have occurred in Drum 68660 due to handling and transport. This type of experiment would be helpful if a predictive thermal runaway model was pursued. The remediation process does entrain the free liquids and liquid in the salt with the Swheat Scoop® material. The water in Drum 68660 was absorbed by Swheat Scoop® as well as entrained in various hydrates and would not be expected to separate from the Swheat Scoop® and hydrates at the resident temperatures over the majority of the lifetime of the drum.

26. Page 27 (first and second paragraph): "The chemical and physical forms of these layers and interfaces are different in chemical reactivity and thermal conductivity. The degree of mixing between the layer of neutralized and sorbed liquid and the layer of nitrate-salt admixture is not known". "The physical configuration at the interface of the neutralized-and-sorbed liquid/Swheat Scoop and the nitrate-salt and mixture/Swheat Scoop layers may have formed a localized region of reactivity leading to the thermal-runway event". Based on our previous question about the materials shown in Fig. 4.2 mixing up, how certain are you about the existence of this localized region?

    There is no absolute certainty about the nature of the interfacial region between the admixture of TEA-neutralized free liquid and Swheat Scoop® and that of the moist nitrate salts and Swheat Scoop®. Bench scale testing indicated that the admixture of TEA-neutralized free liquid and Swheat Scoop® as well as that of the moist nitrate salts and Swheat Scoop® are both reactive. The TAT hypothesized that additional mixing of the two layers, beyond that which occurred during assembly of the drum, could have occurred during post-assembly handling and transport of Drum 68660. Such mixing, if it occurred, increases the possible range of chemical environments and conditions that would support a localized thermal runaway reaction. Note that the thermal chemical model was dependent upon the amount of energy contained in the system and not on the specific location for the initiation. However, the physics of a slow thermal runaway process is characterized by a localized region becoming increasingly reactive and progressing to the runaway condition, which makes one pay attention to areas that are candidates for localized reactivity, such as interfaces of two reactive admixtures.

27. Page 29: Fig. 4.3: The CTH-TIGER model shows localized high temperature after 70 days. Do you consider both heat conduction and convection in the model? Might the high temperature gradient observed in the model be due to unrealistic heat conduction/convection coefficient used?

    For clarity, the CTH-TIGER model was used for the equilibrium calculations and not the determination of the temperature profile in the drum as a function of time. The thermal/chemical model used was SIERRA/Thermal (sometimes referred to as ARIA). Yes, heat conduction, convection, and radiation are considered in the thermal/chemical model. The conductive energy equation with a source term was applied to the waste. Enclosure radiation and free convection were modeled in the head space. The exterior of the drum considered radiative heat loss as well as convective heat loss. Page 82 explains how a radiation boundary temperature of 300 K was used. In addition, a 300 K free convection boundary condition was applied. The conductivity was measured using a surrogate material for the nitrate salts mixed with Swheat Scoop®. The high temperature gradient at ignition is a result of energy being generated faster than the energy is dissipated. The exponential rise in reaction rates with temperature is a result of using temperature dependent Arrhenius-like reaction rates. Conduction/convection coefficients used were deemed realistic and comparable to other scenarios that have been modeled with the Sierra/Thermal code.

28. Page 77: 1st paragraph: The X-ray was used to observe the layer interfaces of different materials in Drum 68660. How did the TAT know the arrangement from top to bottom of these materials?

    The TAT obtained a copy of the radiographic video of Drum 68660 produced at Los Alamos. This video documents the arrangement of the materials in Drum 68660 prior to shipment of the drum to WIPP, consistent with the waste logs and discussions with the operators. In addition to the video, the radiographer's commentary while performing the analysis was documented. The TAT requested the video to be analyzed by an expert at INL to obtain a second interpretation of the Drum 68660 radiographic video. Both interpretations are included in the report (see page 176). From the reports aligning still photographs captured from the video, the TAT was able to align the layers of materials from the bottom to the top of Drum 68660.

29. Page 80: Equation (17) considers the reaction heat sources and heat conduction. How about the convection process?

    Equation (17) is the conductive energy equation and does not include internal convection. Internal convection was not considered relevant because the drum contents were primarily solids, and circulation of air and other free liquids would contribute minimally to heat transfer. However, external convection heat loss was included as part of the boundary conditions. We used a free convection boundary condition as well as a radiative boundary condition. The radiation temperatures as well as the bulk convective temperatures were assumed to be 300 K. The convection coefficient was assumed to be 50 W/m2K. The emissivity of the drum was assumed to be 0.9.

30. Page 94: Are the drum mechanical tests referred to in the literature numerical or physical tests or both?

    The drum mechanical tests referred to in the literature are actual physical tests.

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