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Thermal Analysis of Aged Nitric Acid-soaked Kitty Litter in TRU Waste Drums – 23370

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ABSTRACT

The inadvertent substitution of an organic kitty litter for an inorganic absorbent contributed to the thermal ignition of the transuranic (TRU) waste Drum 68660 at the Waste Isolation Pilot Plant (WIPP) on 2/14/2014. Additional kitty litter remediated nitrate salt (RNS) TRU waste drums have been buried at Waste Control Specialists (WCS) near Andrews, TX, for safety concerns since 2014. To further understand these safety concerns, a previously developed RNS waste model has been calibrated and validated using various experiments at multiple laboratories. The model was also used to predict thermal runaway of Drum 68660 in the WIPP repository as well as the state of the RNS drums at WCS. Measured temperatures are used as boundary conditions for the thermal analysis of the WCS drums. Thermal runaway is not likely to occur provided the RNS drums are adequately vented.

INTRODUCTION

Waste from 1970s and 1980s plutonium recovery operations resulted in nitric acid-washed metal nitrate salts mixed with alpha-emitting radionuclides. Liquids were removed (remediated) with an absorbent. Most of the waste was mixed with an inorganic absorbent, but a fraction was mixed with an organic absorbent (kitty litter). This waste is referred to as remediated nitrate salt (RNS). Runaway reactions within RNS Drum 68660 in the WIPP repository occurred on 2/14/2014 and caused the drum to breach with release of the waste into the repository. The fate of all 313 RNS drums is shown in Fig. 1(a). Of the original 313 RNS drums, 144 drums are currently encapsulated within the WIPP repository (including Drum 68660), 56 drums were re-remediated by dilution with inorganic zeolites, and 113 drums are buried at WCS. The "?" in Fig. 1 implies that the fate of the 113 drums has not yet been determined. The WCS drums are stored within standard waste boxes (SWBs) that are then stored in modular concrete containers (MCCs) as shown schematically in Fig. 1(b).

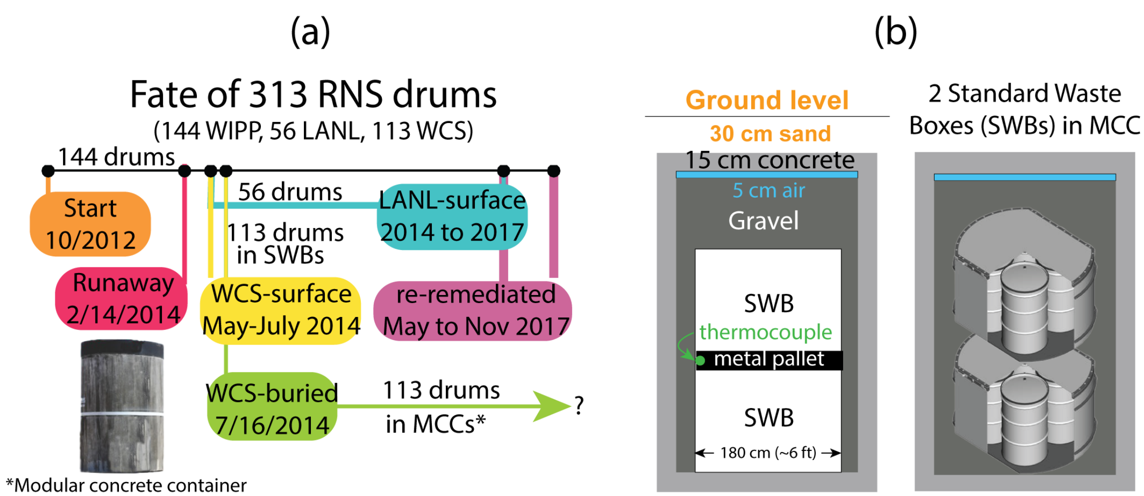

Fig. 1 (a) Fate of RNS drums and (b) cross-section of a modular concrete container (MCC) and two standard waste boxes (SWBs) within an MCC.

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Recently [1], we have modeled decomposing RNS waste using a Universal Cookoff Model (UCM) [2] coupled to a MicroMechanics Pressurization (MMP) model [3]. We obtained model parameters using full-scale RNS drum experiments performed at Los Alamos National Laboratory (LANL) [4] and used the model to simulate thermal runaway of Drum 68660. The waste can be either permeable or impermeable where the decomposition gases are either retained within the waste or the gases can percolate through the waste and exit through the drum vent. In the previous work [1], we investigated the root cause of the Drum 68660 accident. In the current work, we present validation of the waste model using diverse experiments from various laboratories. This model is then used to make predictions of the fate of the 113 RNS drums which are currently buried in MCCs at WCS near Andrews, Texas. We show that vented RNS drums are relatively safe and sealed drums are significantly more dangerous.

MODEL

Details of the UCM/MMP waste decomposition model that is based on a representative waste composition from the contents of Drum 68660 have been presented previously [1]. The processed salts in Drum 68660 were primarily composed of 13 kg of kitty litter known as sWheat Scoop®, 2.7 kg of $Ca(NO_3)_2*4H_2O$, 17.7 kg of $Mg(NO_3)_2*6H_2O$, 3.9 kg of $NaNO_3$, 1.8 kg of $Fe(NO_3)_3*9H_2O$ for a total of 39.1 kg of processed salts. The kitty litter was composed of wheat that likely included starches, cellulose, proteins/enzymes, lipids, minerals, lignin, and other polymeric carbohydrates. A representative single step exothermic reaction for the waste composed of hydrolyzed metal nitrate salts and kitty litter is [5]:

$$C_{2.16}H_{8.64}N_{1.2}O_{7.3}Mg_{0.34}Na_{0.22}Ca_{0.06}Fe_{0.03} \longrightarrow 3.38\ H_2O + 0.45\ CH_4 + 1.2\ CO_2 + 0.6\ N_2 + 0.04\ H_2 + 0.01\ Fe_3O_4 + 0.28\ MgCO_3 + 0.11\ Na_2CO_3 + 0.06\ CaMg(CO_3)_2 + 2.83 \times 10^6 \text{ J/kg} \quad (1)$$

Radioactive decay heat was included in the model by using a 0.15 watt (W) volumetric source ($\dot{q}_{decay}$) for Drum 68660. Decay heat was also considered for the WCS drums calculations. Simulations of the nonradioactive surrogate experiments were performed without the radioactive decay source ($\dot{q}_{decay}$).

The conductive energy equation is solved for temperature leading to runaway:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + h_{r1} r_1 + h_{r1} r_2 + \dot{q}_{decay} \quad (2)$$

In Eq. (2), the terms $\rho C_p \frac{\partial T}{\partial t}$, $\nabla \cdot (k \nabla T)$, $h_{r1} r_1 + h_{r1} r_2$, and $\dot{q}_{decay}$ represent volumetric rates of 1) overall energy change, 2) energy change by conduction, 3) energy change due to moisture evolution and waste decomposition, and 4) energy change caused by radioactive decay, respectively. More information regarding the energy equation is given in [1]. The rate of the reaction, r_2, in Eq. (2) was chosen to match experimental observations of CO_2 and N_2O evolution from RNS drums at LANL where the rates either accelerate or decelerate depending on the confinement and temperature of the waste:

$$r_2 = 1.6 \times 10^{15} \left(\frac{P}{83000}\right)^{5.4} exp\left(\frac{-17360}{T}\right) \left[Waste, \frac{kmol}{m^3}\right]. \quad (3)$$

In Eq. (3), P is pressure (Pa), T is temperature (K), and *Waste* is concentration (kmol/m^3). The rate expression is a first order Arrhenius reaction multiplied by a normalized pressure raised to a power. Pressure accelerates the rate when the waste is confined. Temperature accelerates the rate when the waste is heated. The rate decelerates as the waste composition decreases due to reaction.

Pressure is calculated by assuming the waste is either permeable or impermeable [1, 3]. Decomposition gases within impermeable waste accumulate in isolated defects. In contrast, decomposition gases in permeable waste can percolate through the bed and accumulate within the waste as well as in the headspace volume. If a drum is sealed, the pressure builds up and causes the decomposition rates to accelerate. Pressure acceleration can also occur in vented drums if the waste is impermeable.

MODEL VALIDATION

All the waste material used for validation was surrogate materials without any transuranic elements, except for Drum 68660 which had a volumetric radiation source of 0.15 watts normalized by the waste volume (0.054 m^3). Excluding the radiation source of 0.15 watts would increase the ignition time by about 0.5-2.4% [1], which is within our uncertainty in the predicted ignition time, especially when considering waste permeability. The waste decomposition model was validated with several full-scale LANL drum tests. Full-scale validation with actual waste was performed by predicting thermal runaway in Drum 68660 at WIPP. Validation was also made using small-scale experiments performed at Sandia National Laboratories (SNL) and Pacific Northwest National Laboratory (PNNL) using surrogate waste.

LANL drum experiments

Figure 2 presents predicted temperature profiles for two of the LANL drum experiments. The first experiment shown in Fig. 2(a) is for vented waste that was kept at 298 K (77 ºF) for 93.6 days and then unintentionally increased to 334 K (142 ºF). The temperature change was caused by a power outage that caused the temperature to be reset to a default setpoint of 334 K. The vented drum thermally ignited after a total elapsed time of 97 days (3.4 days after the temperature change). The second experiment shown in Fig. 2(b) is for sealed surrogate waste that was heated from 292 K to 331 K (66-136 ºF) in 74 h when the drum ignited. Figure 2(a) shows the only vented full-scale LANL drum test. A second vented test was attempted, but the vent was restricted due to interference of a sampling cap placed over the vent. The vented experiment matched the data since it was used for calibration. However, the sealed experiment was not used for calibration. The predicted ignition time (76.6 h) using the permeable bed assumption for the sealed LANL drum test was 3.5% higher than the measured ignition time (74 h).

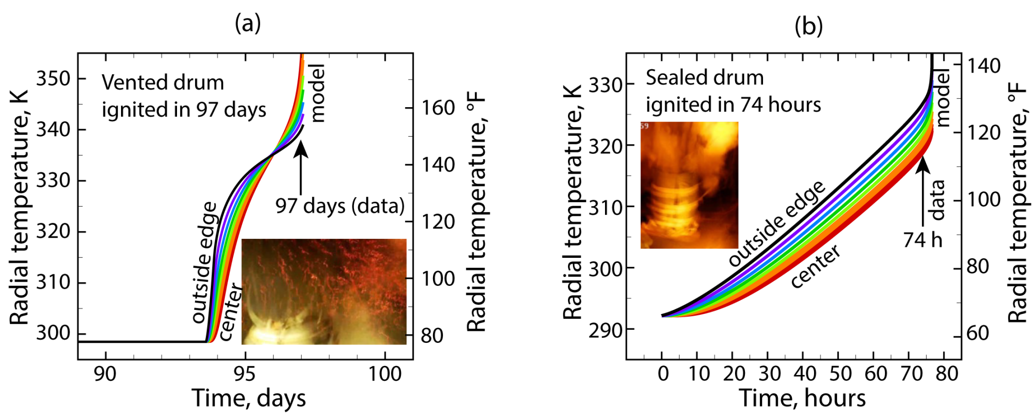

Fig. 2 (a) Vented and (b) sealed LANL drum tests. The inset pictures were taken just after drum failure.

WIPP Drum 68660

Figure 3(a) shows a timeline for Drum 68660 with a lifespan of 73 days. The average drum temperature was about 272 K (30 ºF) or less while above ground. Once the drum was placed in the WIPP repository, the temperature was about 300 K (80 ºF). Here we assume the drum vent became restricted after the flammability test on 1/3/2014 with this being time zero for the calculations. Fig. 3(b) shows the predicted temperatures and pressures for both a permeable bed and an impermeable bed giving ignition occurring between 35.6 days and 62.3 days. The actual ignition time was 44 days as indicated by the gray vertical line in Fig. 3(b).

Figure 3(c) shows the predicted temperature response of a vented Drum 68660 with slight seasonal fluctuations in the repository. The vented predictions indicate that Drum 68660 would not have ignited if the drum had remained vented. These predictions imply that the contents of Drum 68660 were not significantly different than the contents of the other 143 RNS drums that were placed in the repository. The primary difference between Drum 68660 and the other drums is due to a possible restricted vent.

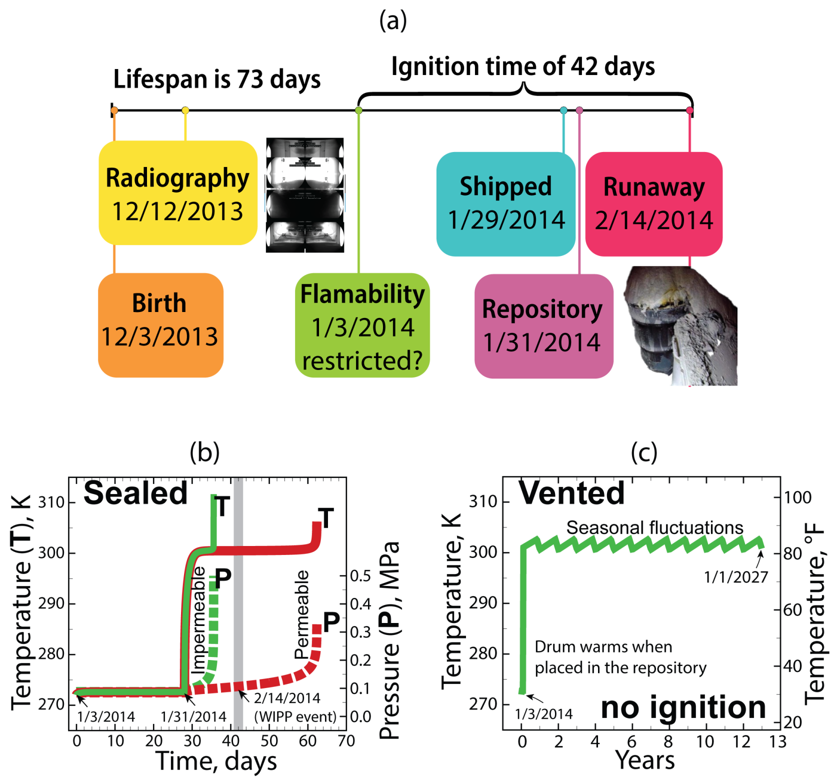

Fig. 3 Drum 68660 (a) timeline and (b) predicted temperatures and pressures using impermeable (green) and permeable (red) bed assumptions. A vented drum prediction is shown in (c). A vented drum is not predicted to ignite.

SITI experiments

Figure 4 presents validation of the waste ignition model using Sandia National Laboratories (SNL) small-scale experiment referred to as the Sandia Instrumented Thermal Ignition (SITI) experiment. Figures 4(a) and 4(b) show a schematic of the SITI apparatus, which consists of two 7.62 cm diameter by 2.29 cm tall aluminum cylinders. A 2.54 cm diameter by 1.27 tall cylinder is machined into each aluminum block. An additional expansion gap is also machined into each of the aluminum cylinders that is 2.22 cm in diameter and 0.16 cm tall. The waste surrogate was confined within this enclosure that also included a vent. Type K thermocouples were placed between the two aluminum halves with the radial location of the thermocouple bead given in Fig. 4(c). Figure 4(d) shows a picture of the kitty litter (sWheat) and the LANL surrogate waste material known as LANL WB4. The LANL WB4 [5] mixture includes 8.4 wt% $Ca(NO_3)_2 {*} 4H_2O$, 0.1 wt% $Cr(NO_3)_3 {*} 9H_2O$, 5.7 wt% $Fe(NO_3)_3 {*} 9H_2O$, 20.6 wt% $Mg(NO_3)_2 {*} 6H_2O$, 36.7 wt% $NaNO_3$, 1.9 wt% $Pb(NO_3)_2$, 1.4 wt% oxalic acid $(COOH)_2$, 0.2 wt% H_2O, and 25 wt% sWheat kitty litter. Figure 4(e) shows the measured and predicted radial temperature for six different surrogate waste materials heated with a 5 K/min temperature ramp from 292 K (66 ºF). Venting is approximated by setting the pressure term to zero, *i.e.,* $\left(\frac{P}{83000}\right)^{5.4} = 0$. For venting, we also neglect the advective loss of enthalpy from outflow, which is small in comparison to the reaction enthalpy. The radiation source is also set to zero, *i.e.,* $\dot{q}_{decay} = 0$. The predicted ignition occurs at 1240 s, which occurs at the same time as the initial measured exotherm for all six of the vented surrogate waste experiments. A second exotherm was observed in some of the SITI experiments. The SITI experiments show that the similarity of the reactive contents outweighs the diversity in the RNS waste.

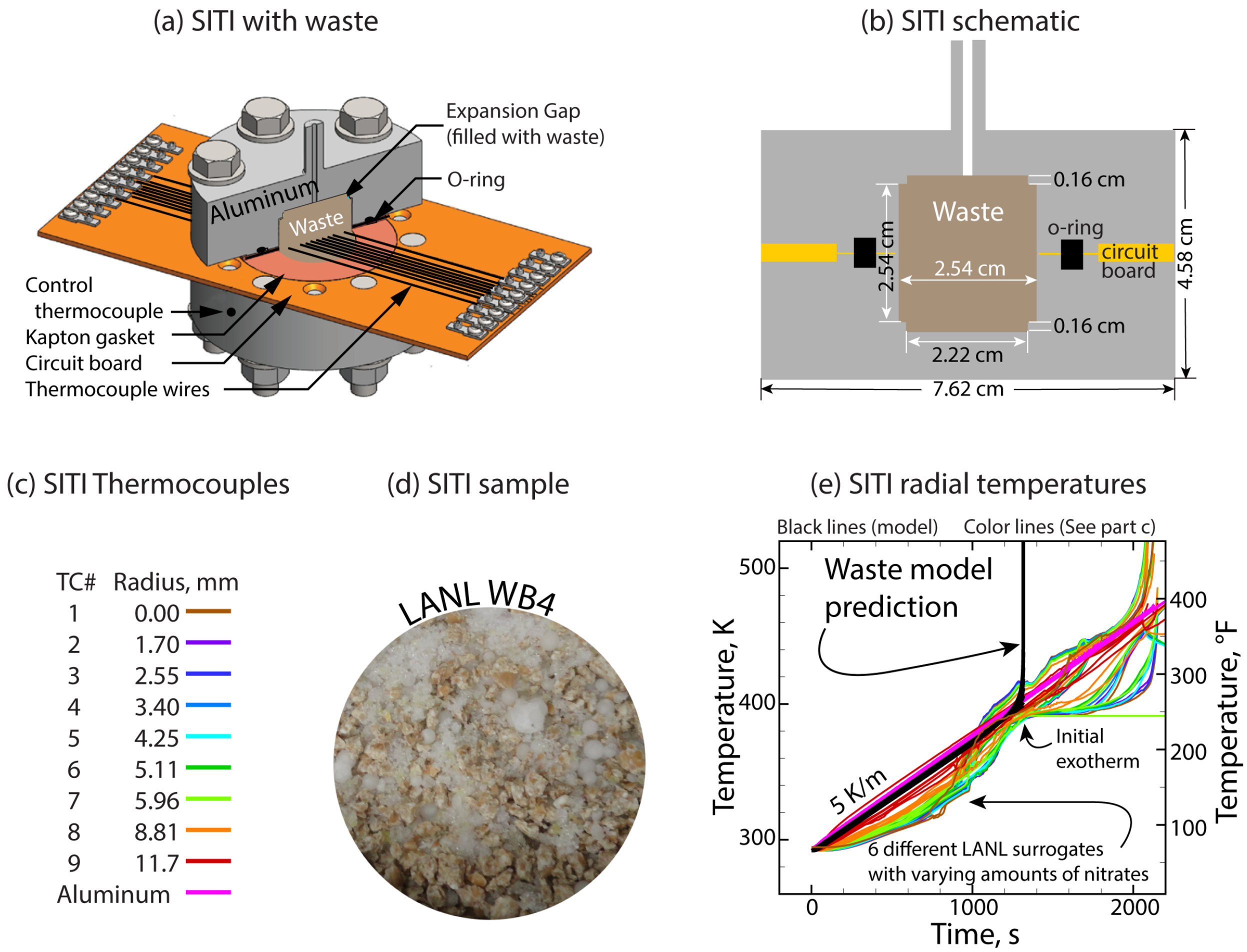

Fig. 4 Vented SITI (a,b) schematics, (c) thermocouple locations, (d) waste picture, and (e) SITI radial temperature profiles corresponding to 6 different LANL waste surrogates with varying amounts of nitrates. Radioactive decay heat is not included in these calculations. The model prediction (black line) corresponds to the initial exotherm in the waste surrogates.

Accelerating rate calorimeter (ARC)

An accelerating rate calorimeter (ARC) was used to determine onset temperatures, temperature rise, as well as heat and pressure generation of surrogate waste compositions. The sample was placed in a closed spherical vessel made of titanium with an internal volume of 9.5 cm^3 and working pressure of 20 MPa (2900 psi). Thermal ignition occurred in two ARC experiments using 1) 7.5-g of dried 3.5 M nitric acid (HNO_3) saturated sWheat [6] and 2) 6.9-g of dried 3.5 M HNO_3 and saturated sWheat [7]. The calorimeter was run using a heat/wait/search mode. The ignition occurred in the two samples when the temperature reached 346 K (163 °F) and 351 K (172 °F), respectively. These two experiments were simulated using a spherical geometry with a waste density of 785 kg/m^3. There was no headspace volume in the first ARC experiment with 7.5-g of waste. However, there was 0.63 cm^3 of headspace volume for the second ARC experiment. Figure 5(a) shows 5 ARC simulations with the temperature ramped from 293 K (68 °F) at five heating rates of 1, 2, 3, 4, and 5 K/min. Constant rate boundary conditions were used due to lack of temperature information on the heat/wait/search mode. The gray box in Fig. 5(a) bounds the measured ignition time that corresponds to the sample reaching 346 K (163 °F) and 351 K (172 °F), respectively. Fig. 5(b) shows the ARC sample containers after each of the experiments in [6, 7].

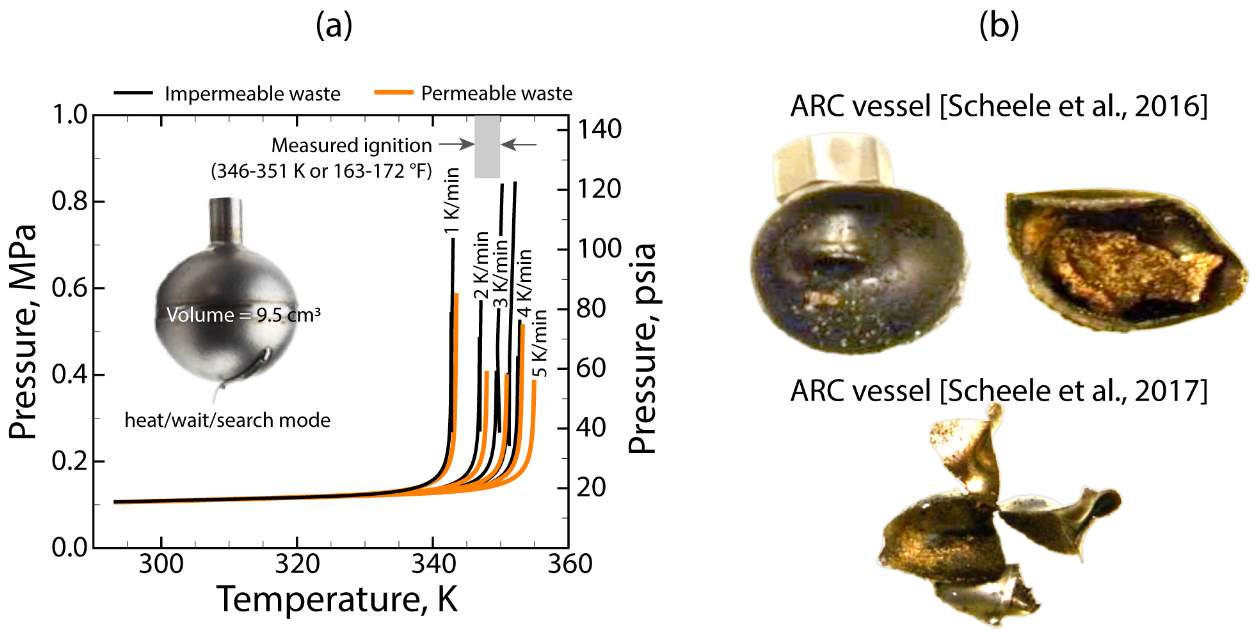

Fig. 5 a) Predicted pressures in ARC calorimeter containing surrogate waste calculated with heating rates varied between 1 K/min and 5 K/min. The inset picture in (a) also shows an ARC container. The pictures in (b) show the ARC container after thermal ignition [6, 7].

MODEL APPLICATION TO AGING WCS DRUMS

Figure 1 shows that 144 RNS drums have been placed in WIPP repository rooms. These rooms have been sealed and the 144 RNS drums are no longer of concern. There were also 56 drums at LANL that were re-remediated by dilution with inert zeolites to make the decomposition reactions endothermic. These drums do not pose a risk for thermal ignition. However, as of 2022, there are 113 RNS drums stored in Standard Waste Boxes (SWBs) that were placed within buried Modular Concrete Containers (MCCs, see Fig. 1b) that could potential thermally ignite. Here we investigate the WCS drums using the waste decomposition model.

Detecting ignition

Figure 6(a) shows temperature decay following thermal runaway at various radial distances from the drum center. The red lines represent temperature at radial distances within the drum; the blue line represents the temperature at the edge of the drum; and the green lines represent temperatures within the surroundings. The domain of the calculations was taken out a radial distance of 91cm. The calculation assumes that all the waste burns and is at the adiabatic flame temperature of 900 K (1200 ºF). The energy within the drum is dissipated via conduction into the surrounding soil. This calculation indicates that the thermocouples should measure a 100 K change in temperature within 10 days of thermal runaway. Figure 6(b-d) show no unusual excursions that are 100 K.

Figure 6(b) provides the temperature data from a thermocouple attached to the metal pallet for a representative MCC, C-276, in 2014. Figure 6(b) also shows the daily high temperatures at Andrews, TX during the same time. The MCC temperatures are slightly higher than the surface temperatures. Figure 6(c) shows the C-276 temperature plotted against the surface temperatures from Andrews Texas in 2014. Clearly, increased reaction occurs in the summer months when the temperatures are higher. Figure 6(d) shows the average temperature of all the MCCs as orange circles. Notice that the year-to-year measured MCC high temperatures decrease over time showing decreasing reactivity. The black line in Fig. 6(d) is a representative boundary temperature that was used for further analysis of the WCS drums over time.

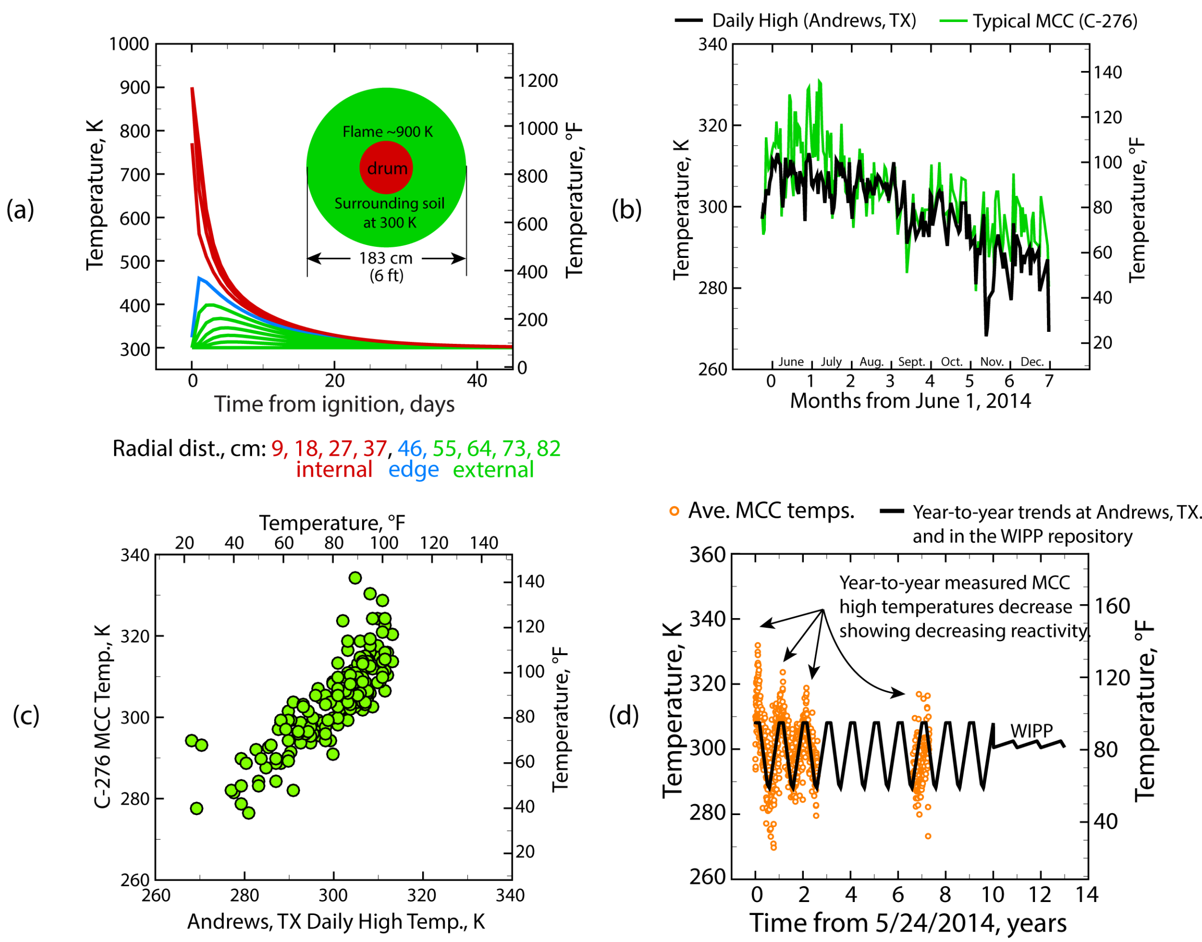

Fig. 6 (a) Model simulations of heat conducting from a drum experiencing thermal runaway to the surrounding soil 183 cm (6 ft.) away. (b) and (c) Comparison of WCS temperature measurements with measurements from a typical MCC (C-276). (d) Year to year measured high temperatures from all MCCs as a function of time. MCCs were stored above ground from May 21, 2014 until July 16, 2014.

Vented ignition in WCS drums

Ignition is not predicted with the boundary condition given by the black line in Fig. 6(d) which has a seasonal high temperature of 308 K (95 °F). If the seasonal high is changed to 327 K (129 °F), thermal excursions are predicted to occur in the summer as shown in Fig. 7(a). However, these excursions are not sufficient to cause thermal ignition. However, if the seasonal high were increased to 328 K (131 °F), thermal ignition would be predicted occur as shown in Fig. 7(b). These calculations indicate that thermal ignition would not occur unless the external temperature reaches 328 K, which is unlikely at WCS. From these simulations, we conclude that thermal runaway in the WCS drums is unlikely in vented drums.

Sealed ignition in WCS drums

Figure 8(a) shows the effects caused by pressure for both an impermeable and a permeable bed of waste within the WCS RNS drums. The acceleration caused by gas restriction and subsequent pressurization is dramatic with ignition occurring within 2 to 12 days. These predictions were made from the time that the drums arrived at WCS in early 2014. Lack of evidence of RNS drum ignition for these drums implies that the flow of the decomposition gases was not restricted as they arrived at WCS and were stored above ground and eventually placed in the MCCs and buried.

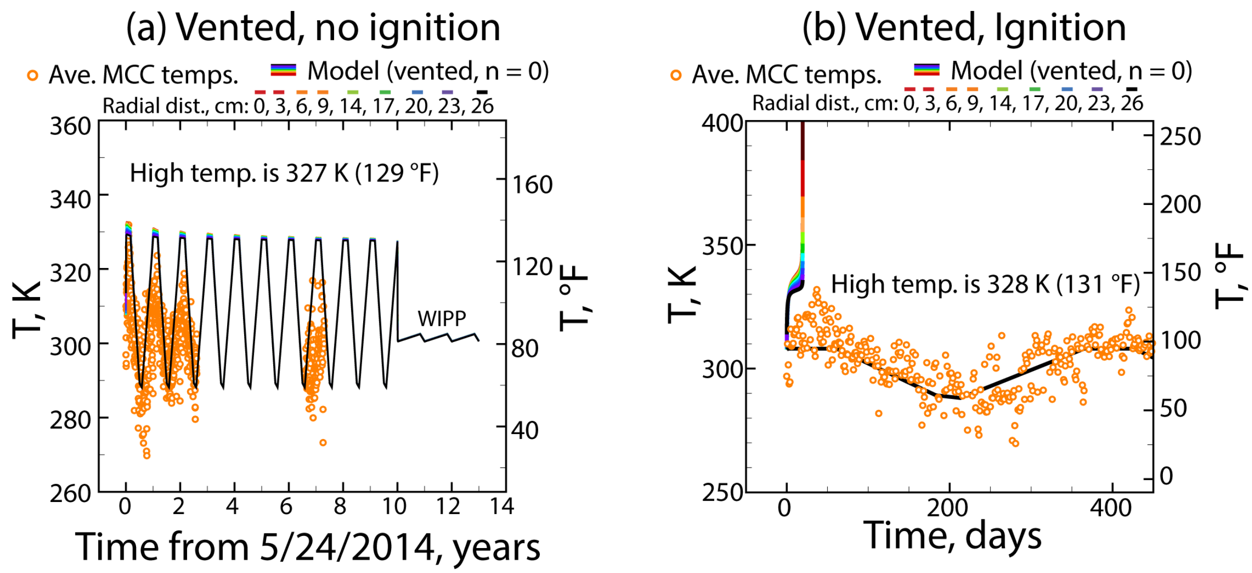

Fig. 7 Simulation of WCS drum with a seasonal high temperature of (a) 327 K and (b) 328 K.

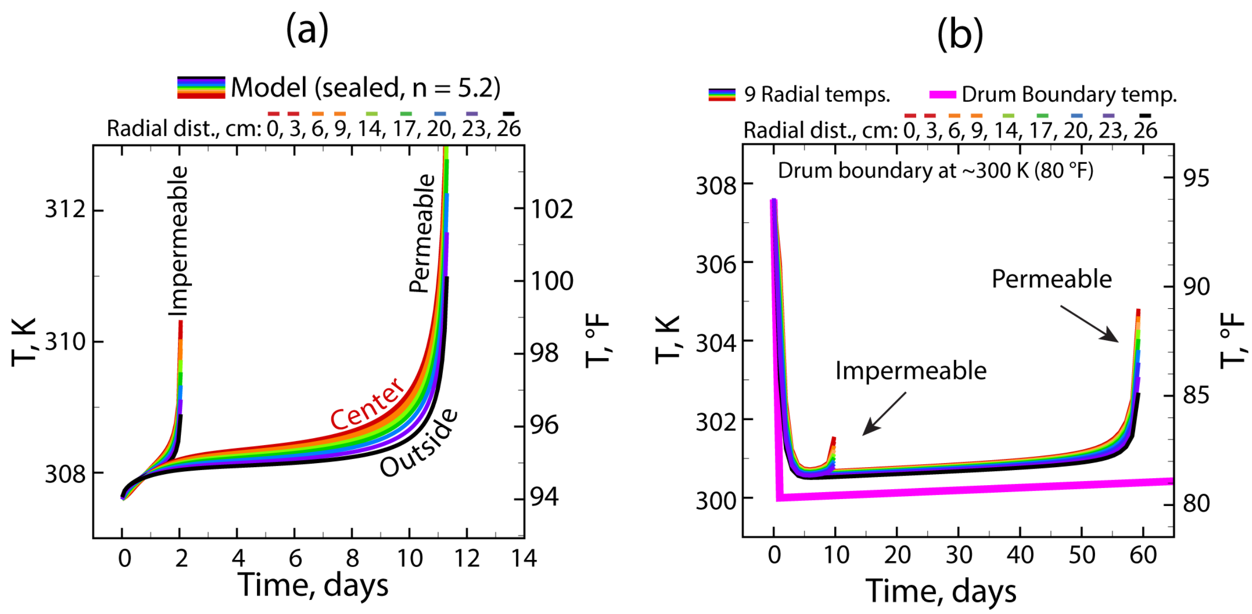

Fig. 8 Predicted ignition for sealed WCS drums. In (a), the drum is sealed just after it arrives at WCS. In (b) a vented WCS drum ($n = 0$) is placed at WIPP after 10 years, and then the drum becomes sealed ($n = 5.4$) Delayed ignition in the aged system in (b) is caused by the concentration of waste being depleted.

Figure 8(b) presents predicted radial temperature profiles for drums that were vented for 10 years and then put into the WIPP repository (at 80 °F) wherein the drums were sealed. After 10 years of decomposition, the waste density changes from 785 kg m^{-3} to 736 kg m^{-3} as the nitric acid and reactive waste are consumed. Predicted ignition times for both impermeable and permeable waste beds were 10 days and 60 days after the initially vented drum is placed into the repository and assumed to be accidentally sealed, respectively. These plots highlight the importance of keeping the RNS drums vented and ensuring gas exchange after emplacement at WIPP.

MODEL SENSITIVITY ANALYSIS

A twenty Latin Hypercube Sample (LHS) uncertainty analysis of Drum 68660 was performed to determine the sensitivity of the predicted ignition time to ten of the input parameters listed in Table 1. The input parameters were assumed to have a uniform distribution over the range listed in Table 1. LHS analysis allows input uncertainty to be efficiently propagated into the model predictions [8]. Table 1 also lists the Pearson correlation coefficient [9] between the input parameters and the predicted runaway time. If the absolute Pearson correlation coefficient is equal to or larger than 0.3, the parameter is considered a primary contributor to the uncertainty. The input parameters that contribute most of the uncertainty in the predicted ignition times were the initial bulk density, the moisture mass fraction, the headspace volume, and the rate multiplier. Figures 9(a) and 9(b) show the edge temperature and pressure for each of the 20 LHS samples, respectively. Figure 9(c) shows the effect of changing the bulk density in impermeable waste. Figure 9(d) shows the effect of the headspace volume when the waste is permeable.

Table 1. Parameters in LHS sensitivity analysis. Last two columns are Pearson correlation coefficients (*r*).

#	Symbol	Description	Range	Mean	r for 68660 impermeable	r for 68660 permeable
1	$C_{p,273}$	Specific heat at 273 K, J/kgK	1090-1210	1150	0.09	0.06
2	$C_{p,343}$	Specific heat at 343 K, J/kgK	1490-1650	1570	0.02	0.01
3	k	Thermal conductivity, W/mK	0.2-0.6	0.4	-0.24	-0.05
4*	r_{bo}	Bulk density, kg/m^3	745-825	785	-0.82*	-0.67*
5	$\dot{q}_{decay}$	Radiation source, W	0.12-0.18	0.15	-0.12	-0.09
6*	V_{ex}	Excess vol. (i.e, headspace), m^3	0.10-0.12	0.11	0.06	0.58*
7	U_{hrxn}	Heat of reaction multiplier	0.95-1.05	1	-0.14	0.03
8*	w_{h2o}	Moisture mass fraction	0-0.066	0.033	-0.39*	-0.24
9*	X	Rate multiplier	0.95-1.05	1	-0.33*	-0.37*
10	e	Emissivity	0.45-0.55	0.5	-0.27	-0.13

*Most important input parameters affecting the uncertainty in the predicted ignition times.

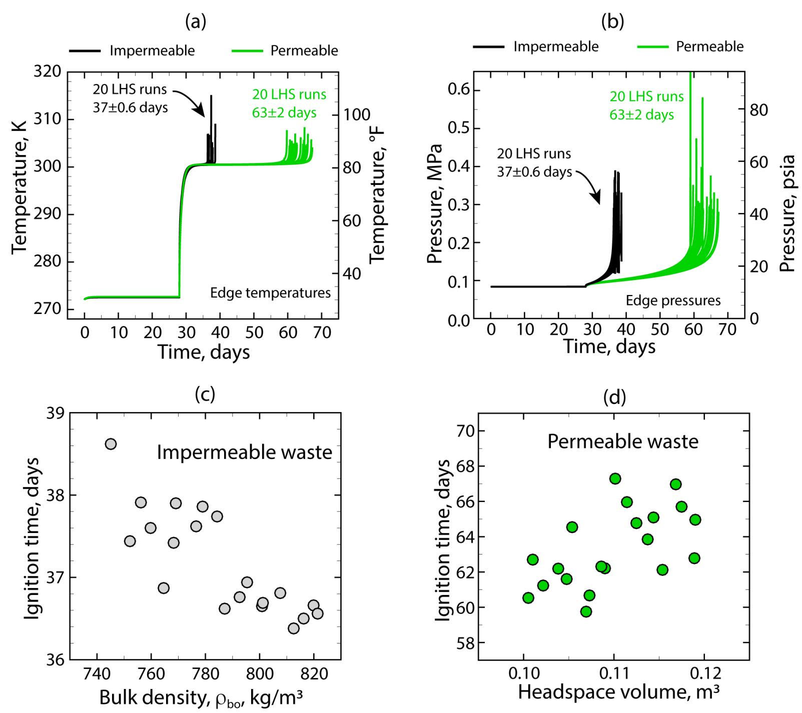

Fig. 9 Predicted (a) temperatures and (b) pressures for each of the 20 LHS runs. In (a) and (b), predictions are shown for both the permeable and impermeable waste. Sensitivity of the predicted ignition time with (c) bulk density for the impermeable waste and (d) headspace volume for the permeable waste.

CONCLUSIONS

A previously developed model of RNS waste has been validated using both small-scale and large-scale experiments at various laboratories that include LANL, SNL, and PNNL. The model was also used to predict thermal runaway of Drum 68660 within the WIPP repository. The specific cause of the 2014 accident involving Drum 68660 has evaded researchers for over 8 years. We believe the root cause of this accident was restriction of the waste drum that resulted in a dramatic acceleration of the nitric acid chemistry and subsequent thermal ignition and radiation dispersal. This view supports the hypothesis that the contents of the RNS drums are not fundamentally different. The model used a simple first-order Arrhenius rate expression that was multiplied by a pressure ratio, $(P/P_o)^{5.4}$. This ratio was set to unity for vented experiments. After the model was validated, it was used to predict the state of RNS drums that are currently (as of 2022) being stored at the WCS facility near Andrews, Texas. The model predicts that the vented drums are relatively safe and that sealed drums could ignite within a short period of time.

REFERENCES

[1] M. L. Hobbs, P. F. Britt, D. T. Hobbs, M. J. Kaneshige, M. Minette, J. Mintz, F. M. Pennebaker, G. R. Parker Jr., R. Pierce, D. M. Rosenberg, J. Schwantes and A. Williams, "Thermal runaway of nitric acid-soaked kitty litter in transuranic waste," *Process Safety and Environmental Protection,* vol. 167, pp. 543-549, 2022.

[2] M. L. Hobbs, M. J. Kaneshige and W. W. Erikson, "A universal cookoff model for explosives," in *50th International Annual Conference of the Fraunhofer ICT, Energetic Materials--Past, Present and Future*, Karlsruhe, 2019.

[3] M. L. Hobbs, J. A. Brown, M. J. Kaneshige and C. Aviles-Ramos, "A Micromechanics Pressurization Model for Cookoff," *Propellants Explos. Pyrotech.,* vol. 47, no. 2, pp. 1-15, 2022.

[4] G. R. J. Parker, M. D. Holmes, E. M. Heatwole, P. Leonard and C. P. Leibman, "Drum-scale Testing of the Thermolytic Response of a Remediated Nitrate Salts (RNS) Surrogate Waste Mixture," Los Alamos National Laboratory Report LA-CP-16-20038, Los Alamos, 2016.

[5] D. L. Wilson, M. L. Baker, B. R. Hart, J. E. Marra, J. M. Schwantes, P. E. Shoemaker, M. Knotek, T. A. Michalske and D. Klaus, "Waste Isolation Pilot Plant Technical Assessment Team Report," Savannah River National Laboratory, Report SRNL-RP-2014-01198, Aiken, 2015.

[6] R. D. Scheele, M. J. Minette, B. K. McNamara and J. M. Schwantes, "Thermochemical Reactivity Hazards of TRU Waste Constituents-16075," in *WM2016 Conference*, Phoenix, 2016.

[7] R. D. Scheele, B. K. McNamara, J. M. Schwantes, D. T. Hobbs, M. J. Minette and C. A. Barrett, "Thermoanalytical investigation of the reactions causing the transuranic waste drum breach that occurred in the Waste Isolation Pilot Plant," *Thermochimica Acta,* pp. 76-87, 2017.

[8] M. D. McKay, R. J. Beckman and W. J. Conover, "A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code," *Technometric,* vol. 21, pp. 239-245, 1979.

[9] J. L. Rodgers and W. A. Nicewander, "Thirteen Ways to Look at the Correlation Coefficient," *The American Statistician,* vol. 42, pp. 59-66, 1988.

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