MARY KAY O'CONNOR PROCESS SAFETY CENTER
TEXAS A&M ENGINEERING EXPERIMENT STATION

19th Annual International Symposium
October 25-27, 2016 • College Station, Texas

Transient Large-Scale Chlorine Releases in the Jack Rabbit II Field Tests: Rainout Source Data Analysis

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Abstract

Sponsored by the Chemical Security Analysis Center (CSAC) of the U.S. Department of Homeland Security, the Defense Threat Reduction Agency (DTRA) of the U.S. Department of Defense, and Transport Canada, the Jack Rabbit II tests were designed to release liquid chlorine at ambient temperature in quantities of 5 to 20 T for the purpose of quantifying the behavior and hazards of catastrophic chlorine releases at scales represented by rail and truck transport vessels. Phase 1 of the two-year testing campaign was conducted at Dugway Proving Ground, Utah, in August and September of 2015. Five successful field trials were conducted in which chlorine was released in quantities of 5 to 10 tons through a 6-inch circular breach in the tank and directed vertically downward at 1 m elevation over a concrete pad. In 2016, four trials were conducted with three releases of nominally 10 T at different orientations and a single release of 20 T vertically downward. Data from the 2015 tests are available. This paper summarizes preliminary analysis of the available data from the concrete pad including analysis of the temperature measurements below and grade in the concrete pad.

Introduction

Initiated by the U.S. Department of Homeland Security (DHS) Transportation Security Administration (TSA) Freight Rail HAZMAT division, the Department of Homeland Security (DHS) Chemical Security Analysis Center (CSAC) planned and conducted the Jack Rabbit (I) test series, a series of mid-sized field tests on the two highest priority toxic inhalation hazard (TIH) materials, chlorine and anhydrous ammonia (Fox and Storwold, 2011). The one and two (short) ton releases were conducted at the Dugway Proving Grounds (DPG) in April and May of 2010 for the overall goal of improving the understanding of the consequences of large scale TIH releases. Key findings of the tests were the significant persistence of the denser-than-air clouds formed during the release (more prevalent with increased release size) (Hanna et al., 2012) and the extent to which chlorine removal could mitigate the impact of a release (Hearn et al., 2012).

As a continuation of the previous tests, the Jack Rabbit II (JRII) test program was started in 2014 to focus on large scale, controlled chlorine field experiments representative of releases from railcars and tank-trucks (5 to 20 tons). The broad scientific goals of the test program are to collect data on the release source, cloud transport and dispersion, chemical reactions with the environment (including potential mitigation effects), exposure effects on equipment and infrastructure, and effect of releases within a mock urban test environment including indoor infiltration. In addition, the program will provide data, training materials, and guidance for improved emergency response efforts and support the Homeland Security Enterprise by providing quality-assured data and scientifically-based guidance to partners and stakeholders to address assessment of TIH hazards.

Preparations for the tests were organized using a series of working groups to handle specific aspects of the program including:

- Data Quality Working Group
- Instrumentation Working Group
- Mock Urban and Indoor Environment Working Group
- Modeling Working Group
- Dissemination and Near Source Working Group

Oversight and coordination of activities of the working groups is through the program's Scientific Advisory Group (SAG) with final approval by CSAC.

The dissemination system consisted of a custom-built vessel (disseminator) and support system including load cells for continuous force (mass) measurement during the release. The system was centered on a 25 m diameter concrete pad approximately 6 in deep designed to collect liquid rainout and to protect the gravel pad constructed on the playa at DPG from the chlorine aerosol jet anticipated during the tests. The intention was for the concrete pad to be level and flat, but the process of pouring the large pad at the remote testing location resulted in imperfections such as low or high areas on the pad. The process was also made more difficult because of the desire to not have cracks or expansion joints were chlorine could seep below the pad creating operational issues. A 1 in lip was installed at the edge of the pad to keep liquid from flowing onto the gravel pad. Details of the vessel, support system, and vessel instrumentation are reported elsewhere (Spicer et al, 2016).

At this point, the tests conducted in 2015 and 2016 have been completed, but data from the 2016 tests has yet to be released. Table 1 summarizes the tests conducted during the 2015 season. All times are local times (MST). The release time is taken to be the time in the data acquisition system when the load cells reflect a significant change. In Table 1, the chlorine mass released was calculated from the difference between the four vertical load cells before and after the release. In Trial 5, the data acquisition system failed during the release, so the final (tare) mass was taken to be the average of the final mass in the previous four tests.

Table 1. Jack Rabbit II Test Summary for 2015 Trials

Trial	Date	Release Time	Mass Released (T)	Wind Direction	Wind Speed (m/s)	Air Temperature (°C)	Pressure (Pa)	Relative Humidity (%)
1	8/24	7:35:45.50	5.01	147°	2.0	17.7	87400	39.2
2	8/28	9:24:20.00	9.03	158°	4.2	22.7	87500	32.8
3	8/29	7:56:55.31	5.03	169°	3.9	22.7	87100	30.2
4	9/1	8:38:47.05	7.73	183°	2.3	22.6	86900	26.8
5	9/3	7:28:17.26	9.20	182°	2.7	22.2	86700	26.5

In the 2015 and 2016 tests, measurements were made in an attempt to quantify the rainout on the concrete pad at three measurement stations (Figure 1). Locations labeled Pad 1 and 2 included thermocouples (Type K, 24 AWG) above grade and embedded in the concrete pad along with Guided Wave Radar (GWR) instruments. This was a nonstandard use of the GWR in an attempt to quantify the anticipated rainout, but the liquid rainout was insufficient to be measured by the GWR. Preliminary calculations had indicated that a significant amount of rainout was predicted by several models, which prompted the addition of the GWR in the event that rainout was significant. At Pad 3, only thermocouples were deployed. Planning for the 2016 tests included the addition of an inner ring (28 ft diameter, 12 in high) on a single test in an attempt to trap the rainout so that it could be measured with the GWR at Pad 2, but this test was unable to be conducted because of weather and scheduling issues. This paper discusses the temperature measurements made in the concrete pad during the 2015 tests.

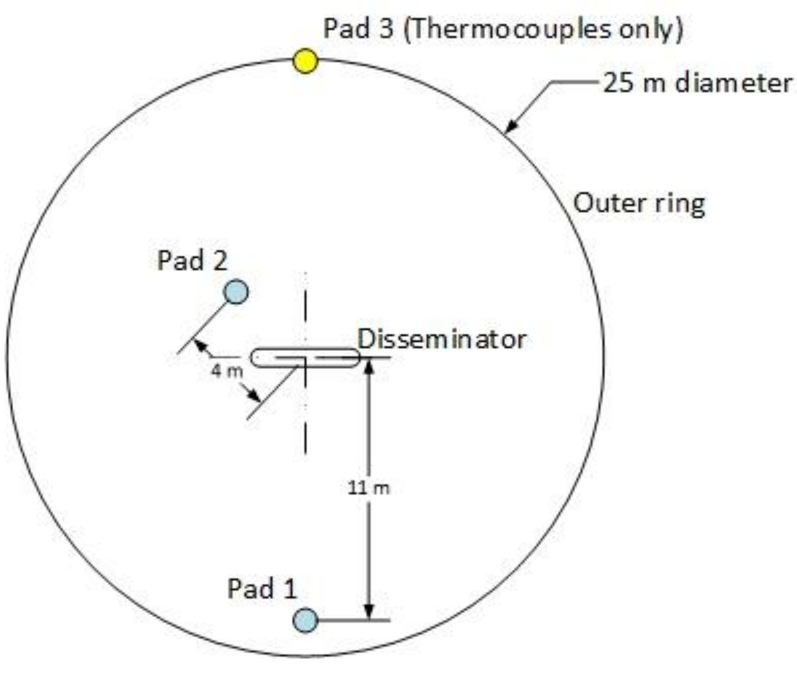

Figure 1. Overhead view of Disseminator on concrete pad showing measurement locations

Temperature Measurements in the Concrete Pad during 2015 Testing

At all three pad locations, thermocouples were placed below grade by making vertical cuts in the concrete pad, placing the thermocouple at the specified depth, and (re-)filling with concrete. To reduce the potential impact of thermal conduction along the length of the wire, the thermocouple wire was placed below grade in the vertical cut for approximately 10 cm so that the wire lead was (roughly) horizontal in the vertical cut. One wire was placed in each vertical cut, and vertical cuts were spaced roughly 10 cm apart in parallel. In addition to a thermocouple similarly placed at the concrete surface (so that the wire lead was below grade), thermocouples were placed at depths of 0.03, 0.06, 0.09, 0.15, and 0.22 mm. (Thermocouples above grade were at elevations of 0.5, 1, 2.5, 10, 40, 100, 200, and 300 cm.)

Figure 2 shows the surface temperature measured at all three Pad locations in Trial 2. (Trial 2 was chosen as an example because it was the largest mass released in 2015 testing with data collection; the data acquisition system failed during Trial 5 shortly after the release started.) Figure 2 shows that the temperatures dropped rapidly after the start of the release and quickly fell to the boiling point at ambient pressure (-37.2 °C). Although data was intended to be collected at 100 Hz, data acquisition issues caused data to be recorded at roughly 0.5 Hz (once every 2 s).

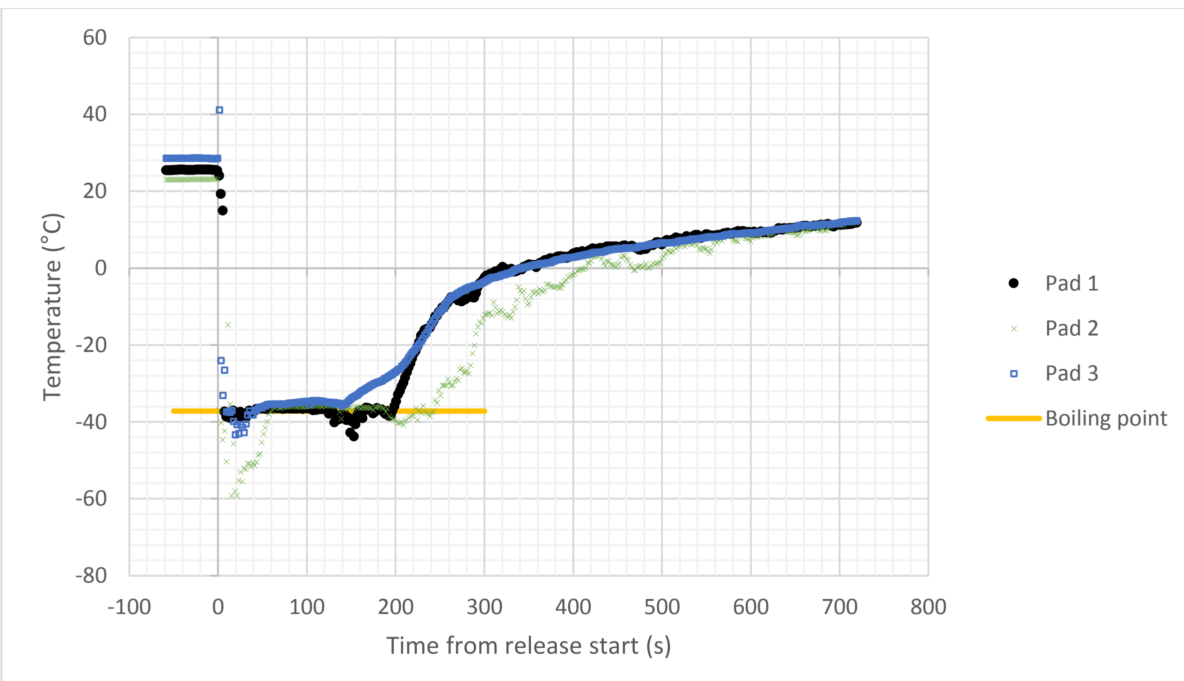

Figure 2. Surface temperature measurements at all Pad locations as a function of time in Trial 2.

Figure 3 shows the measured temperature as a function of depth and time at Pad 1. The temperatures are initially ordered as would be expected with coldest temperatures near the surface. Note that the release duration for Trial 2 was roughly 53 s (based on load cell measurements), and the surface temperature at Pad 1 was near the boiling point until roughly 200 s indicating liquid likely present until the ground surface temperature starts to increase. All of the measurements (except at 6 mm) also show the effect of continuing to cool after the cold surface temperature starts to warm to ambient temperature. A plausible explanation of these measurements would be that the 6 mm thermocouple was at a local high spot in the concrete so that surface liquid evaporated away from this location before the area where the other thermocouples were placed. Consequently, the measurements at 6 mm will be excluded from further analysis at Pad 1.

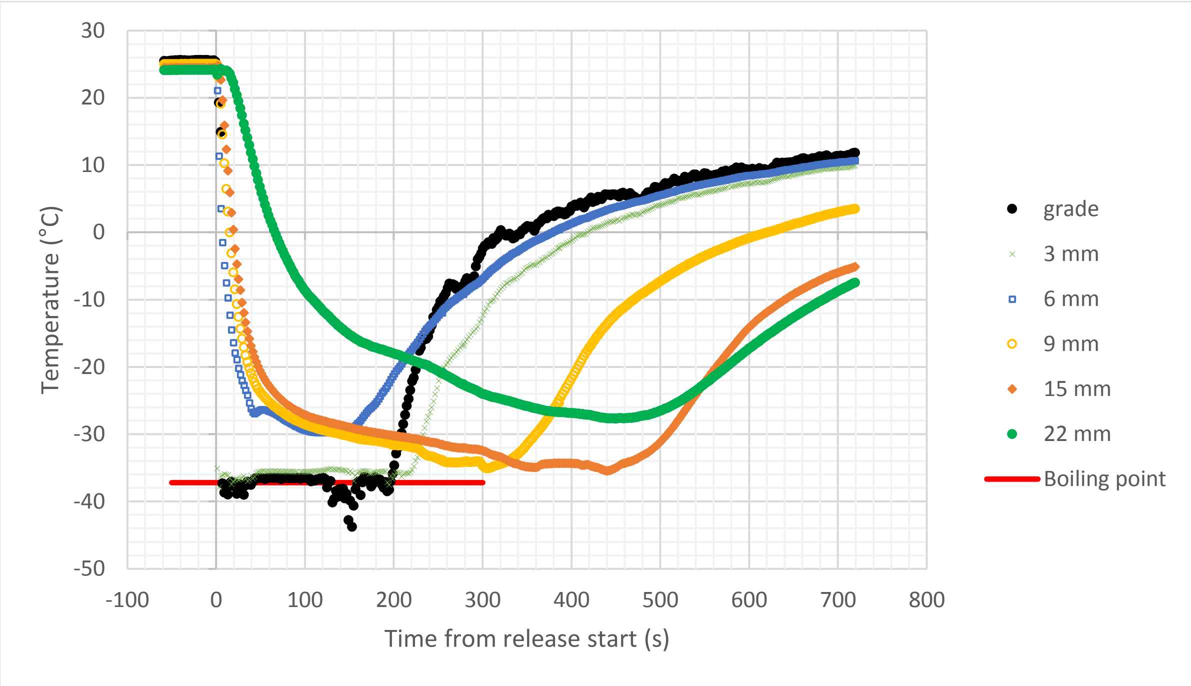

Figure 3. Measured temperature as a function of depth in the concrete pad at Pad 1.

Figure 4 shows the measured temperature as a function of depth and time at Pad 2. The measurements at 6 and 22 mm show the temperature dropping to the boiling point almost immediately indicating that there was likely liquid infiltration to the thermocouple along the length of the wire. The 6 mm measurements are consistent with the surface temperature measurements during the release indicating this thermocouple was essentially recording temperatures at the concrete surface. Although it is difficult to determine from the plot, the measurements at 3 and 9 mm are essentially identical likely indicating an issue with thermocouple placement. Also, the measurement at 15 mm shows a lower minimum temperature than was recorded at 3 and 9 mm. As at Pad 1, the measured surface temperature is near the boiling point for roughly 200 s longer than the release duration. Note that the surface temperature drops below the boiling point while the release is ongoing. Temperatures below the boiling point can be observed due to liquid phase chlorine contacting air (vapor/liquid equilibria causes the liquid to cool below its boiling point). Close inspection of Figure 4 shows that the temperatures below the boiling point last for the duration of the release (53 s) after which time the temperature rises slightly above the boiling point before falling to the normal boiling point at around 130 s. Furthermore, the measurements at 22 mm show the temperature increasing from the boiling liquid temperature at roughly 60 s after the release started.

A plausible explanation of these temperatures is that during the release, liquid chlorine is in contact with air around Pad 2 but the liquid is only in a thin film which changes phase shortly after the release is complete. Immediately after the release stops, cold gas is present at Pad 3, but as time goes along, some chlorine aerosol flows back over the area due to unevenness in the concrete pad. Measurements at 3, 9, and 15 mm are starting to show warmer temperatures which would be consistent with high heat transfer rates during the release with heat transfer rates significantly declining after the release stops. Consequently, the surface temperature measurement seems reliable at Pad 2, and the measurements at 3, 9, and 15 mm seem plausible but at different locations which may not be easily determined.

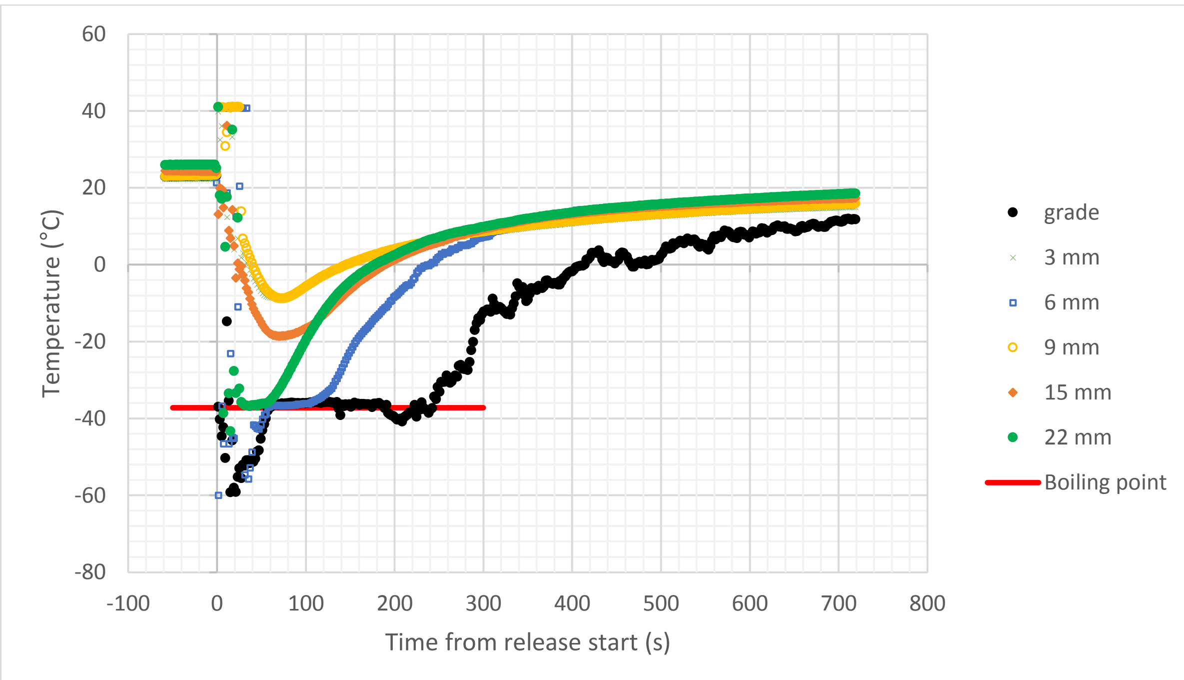

Figure 4. Measured temperature as a function of depth in the concrete pad at Pad 2.

Figure 5 shows the measured temperature as a function of depth and time at Pad 3. The measurement at 22 mm again shows the temperature dropping to the boiling point almost immediately indicating that there was likely liquid infiltration to the thermocouple along the length of the wire. As at Pad 2, the measurements at 22 mm show the temperature increasing from the boiling liquid temperature at roughly 60 s after the release started. The measured surface temperature also rises above the boiling point at the end of the release, and this is consistent with the fact that Pad 3 is the farthest measurement location from the release point. The measurements at 3, 9, and 15 mm seem to be consistent with liquid being present up until the end of the release and quickly evaporating after the release is complete. The measurements at 6 mm seem unusually noisy and erratic. Consequently, the measurements at 6 and 22 mm will be excluded from further analysis at Pad 3.

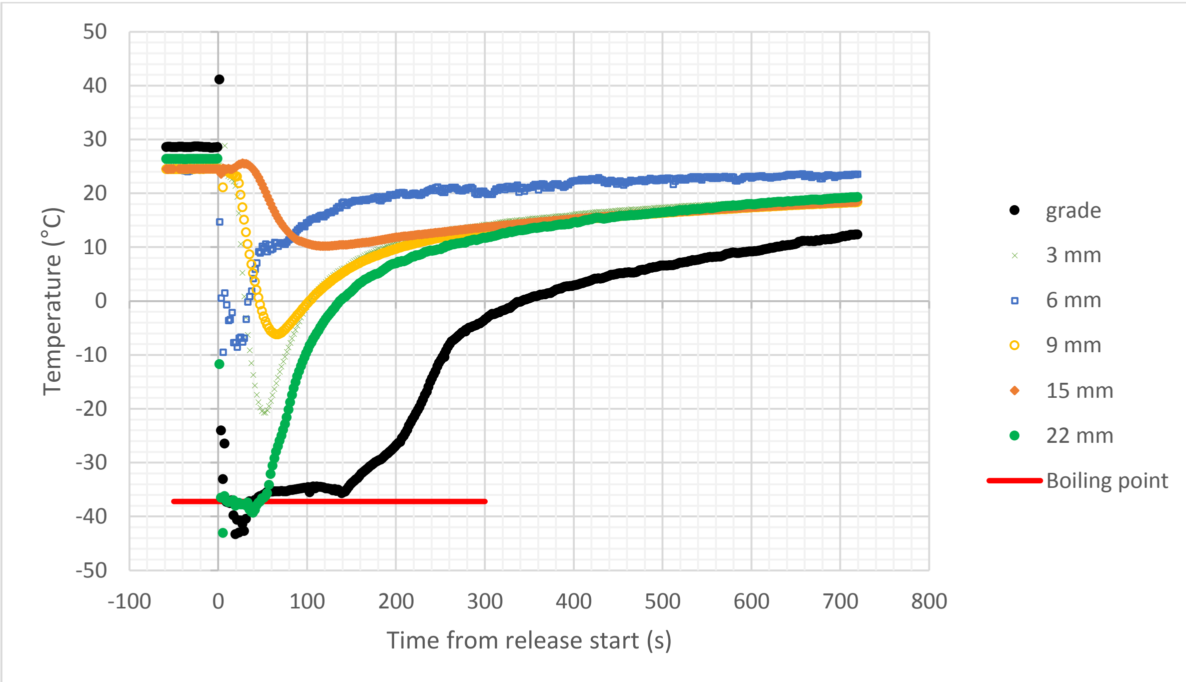

Figure 5. Measured temperature as a function of depth in the concrete pad at Pad 3.

Table 2 summarizes the findings as considered here for Trial 2. The consistency of the thermocouple readings across all tests need to also be considered, but this exercise in incomplete at present. (For example, a thermocouple with questioned measurements would not be expected to spontaneously produce more reliable measurements in a subsequent trial.)

Table 2. Summary of observations taken from temperature measurements in the concrete pad taken during Trial 2.

Measurement Location	Valid Temperature Measurement Depths (mm)	Liquid Chlorine Present
Pad 1	grade, 3, 9, 15, 22	substantial liquid puddle lasting 200 s
Pad 2	grade (3, 9, 15)*	thin liquid puddle that evaporates soon after the release is complete
Pad 3	grade, 3, 9, 15	thin liquid puddle that evaporates soon after the release is complete

* large uncertainty in the depth of these measurements

Analysis of Temperature Measurements

The theory for calculating the temperature profile in a solid is well established. One-dimensional heat transfer in a solid is governed by the Fourier Equation:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho C_p}\frac{\partial^2 T}{\partial^2 x} = \alpha \frac{\partial^2 T}{\partial^2 x} \tag{1}$$

where k is the thermal conductivity, C_p is the heat capacity, ρ is the density, α is the thermal diffusivity ($k/(\rho C_p)$), and T is a function of depth x and time t. (For simplicity, the depth $x \geq 0$.) As is shown in the data, the surface temperature remains constant (T(x=0) = -37.2°C) when liquid appears to be present, but after the liquid evaporates, a convective boundary condition should be applied

$$q''(t) = -k \left.\frac{\partial T}{\partial x}\right|_{x=0} = h(T_a\text{-}T_0) \tag{2}$$

where q″ is the surface heat flux, h is a convective heat transfer coefficient, T_a is the ambient temperature, and T_0 is the surface temperature. Equation (1) can be rewritten as a system of ordinary differential equations on a spatial grid with temperatures $T_i(t)$ using a second order approximation to the spatial derivative:

$$\begin{aligned}\frac{dT_i}{dt} &= \alpha \frac{d^2 T}{d^2 x} \\ &= \alpha \left(\frac{2T_{i+1}}{(x_{i+1}\text{-}x_i)(x_{i+1}\text{-}x_{i\text{-}1})} + \frac{2T_i}{(x_{i+1}\text{-}x_i)(x_i\text{-}x_{i\text{-}1})}\right. \\ &\quad \left. + \frac{2T_{i\text{-}1}}{(x_{i+1}\text{-}x_{i\text{-}1})(x_i\text{-}x_{i\text{-}1})}\right)\end{aligned} \tag{3}$$

for all internal locations in the solid (i = 0 to n). At the surface after convection applies, the time derivative of the surface temperature is approximated as

$$\frac{dT_0}{dt} \cong \frac{\alpha}{\Delta x}\left(\left.\frac{dT}{dx}\right|_1 - \left.\frac{dT}{dx}\right|_0\right) = \frac{\alpha}{\Delta x}\left(\frac{T_2\text{-}T_0}{2\Delta x} + \frac{h}{k}(T_a\text{-}T_0)\right) \tag{4}$$

where Δx is for a uniform grid. At the (internal) edge of the domain, an insulating boundary condition can be applied in a similar fashion

$$\frac{dT_n}{dt} \cong \frac{\alpha}{\Delta x}\left(\left.\frac{dT}{dx}\right|_n - \left.\frac{dT}{dx}\right|_{n\text{-}1}\right) = -\frac{\alpha}{2\Delta x^2}(T_n\text{-}T_{n\text{-}2}) \tag{5}$$

A numerical solution was developed for the system of ordinary differential equations in MATLAB.

Using generic properties for concrete (k = 1.65 W/mK, ρ = 2300 kg/m^3, Cp = 880 J/kgK, and α = 8.2×10^{-7} m^2/s), the equations can easily be solved on an evenly spaced 1 mm grid (so $x_{i+1} - x_i$ = +1 mm).

Based on the discussion above, Pad 1 was simulated with a constant temperature boundary condition for 200 s. The fact that temperatures farther into the concrete continue to drop after the surface temperature begins to warm can qualitatively be reproduced if the concrete pad was thinner in this area. The simulation shown in Figure 6 was made assuming h = 100 W/mK (high to bring the surface temperature to approximate the data and a very thin concrete layer (23 mm). The simulation shows similar general characteristics as the data, but there seem to be characteristics of the data that are currently not being modeled properly.

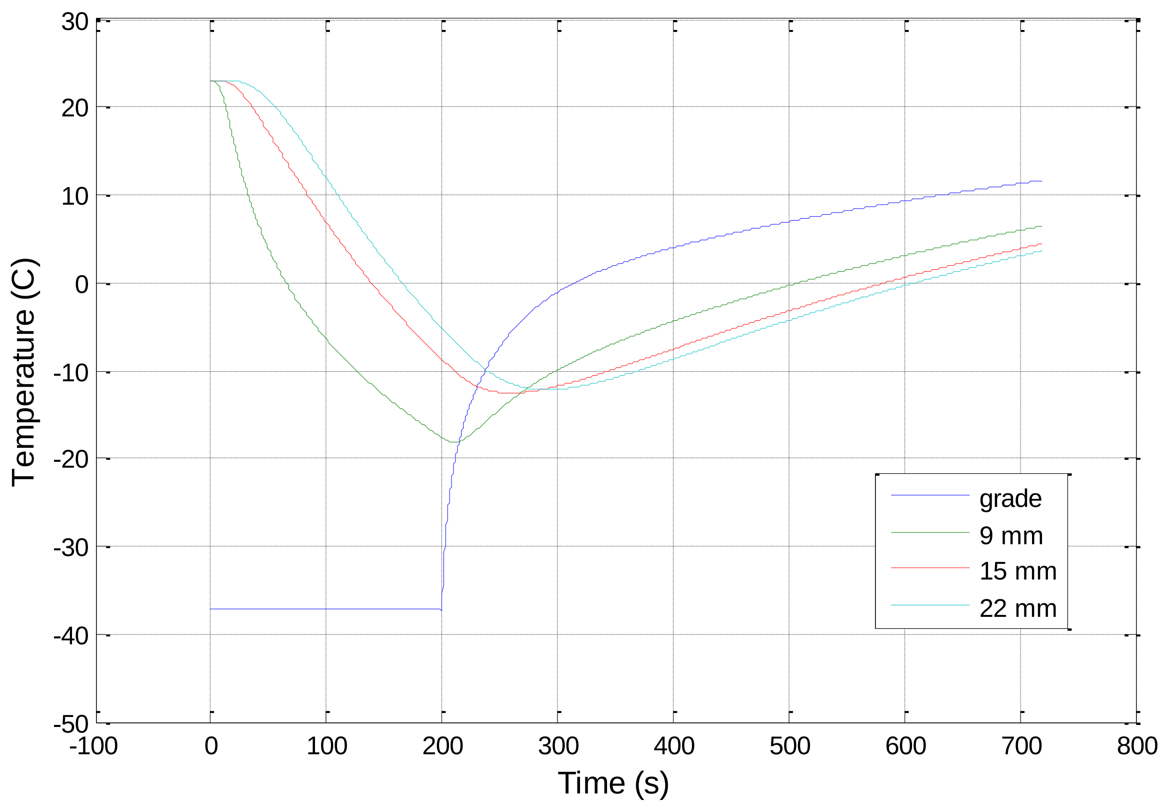

Figure 6. Simulation of Pad 1 temperatures in Trial 2 for selected measurement locations.

Based on the discussion above, Pad 3 was simulated with a constant temperature boundary condition for 60 s. The simulation shown in Figure 7 was made assuming h = 10 W/mK and the anticipated concrete thickness of 6 in. The simulation shows quite similar general characteristics as the data, but there seem to be characteristics of the data that are currently not being modeled properly. Minimum temperatures and the times at which they occur are consistent with observations.

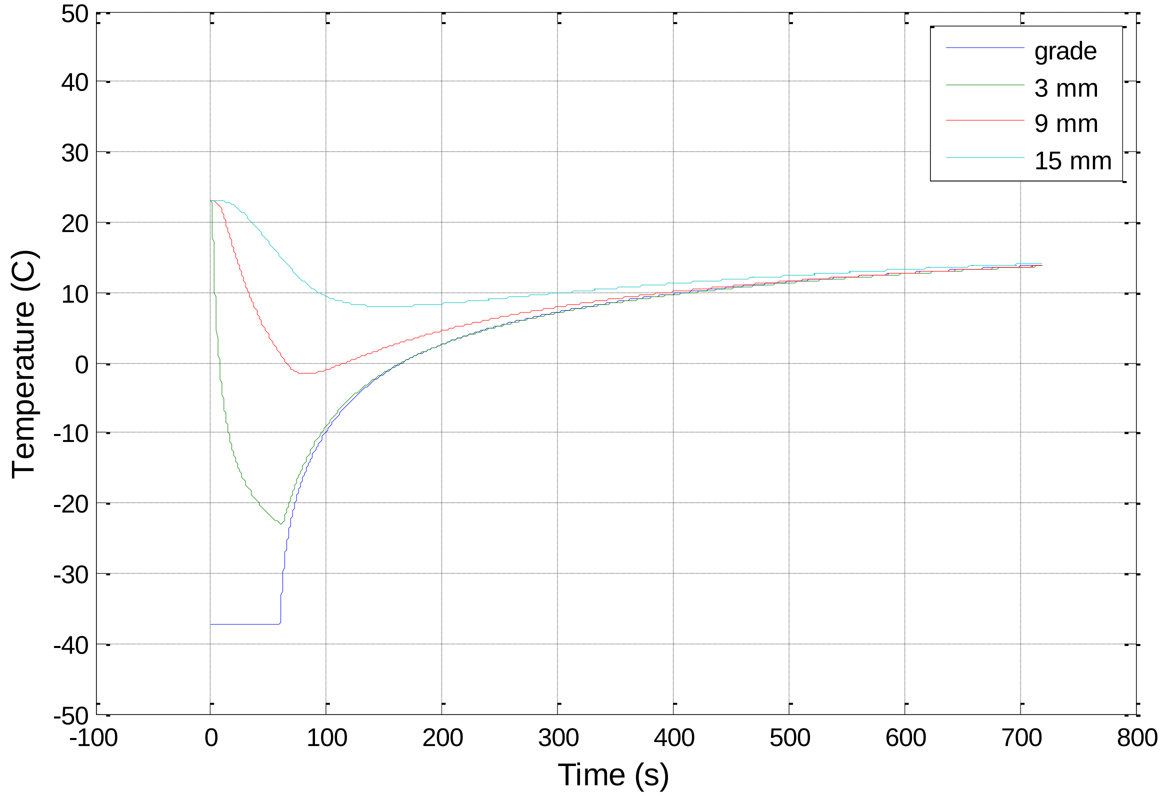

Figure 7. Simulation of Pad 3 temperatures in Trial 2 for selected measurement locations.

A request has been made to obtain samples of concrete from the pad so that properties (density, thermal diffusivity, and heat capacity) can be determined.

Test Program Data Availability

The 2015 test program data is currently available, but the 2016 test program data set is currently going through a verification and validation process. At this point, all instruments have been subjected to a post-test calibration process for the 2015 tests, and all instruments were within calibration limits.

There are plans to make all data from the test program available to the public via the Homeland Security Information Network (HSIN) web site. HSIN access is based on a nomination/acceptance process into a Community of Interest (COI). To begin the process, email HSIN.outreach@hq.dhs.gov with your full name and email address including the requested COI (Chemical) and the reason for access: “To become a member of the Jack Rabbit II community to have access to the information and data from the test program.”

Conclusions

Phase I of the Jack Rabbit II test program has been completed with controlled releases of liquid chlorine at ambient temperature for the purpose of quantifying the behavior and hazards of catastrophic chlorine releases at scales represented by rail and truck transport vessels. Five successful field trials were conducted in which chlorine was released in quantities of 5 to 10 tons through a 6-inch circular breach in the disseminator vessel and directed vertically downward at 1 m elevation over a concrete pad in a mock urban environment.

This paper summarized the measurements made to quantify liquid rainout during the 2015 tests. Temperature measurements support visual observations that some limited liquid rainout was observed. The quantity rained out is insignificant in comparison with the total mass of chlorine released, but liquid rained out during the release will be sufficient to pose issues for people near the release point.

Acknowledgements

This field test program was sponsored by the Chemical Security Analysis Center (CSAC) of the U.S. Department of Homeland Security (DHS), the Defense Threat Reduction Agency (DTRA) of the U.S. Department of Defense, and Transport Canada. In addition to the program's Dissemination and Near Source Working Group, we acknowledge the contribution of many people who planned and conducted the first season of tests: DHS CSAC including Adolfo Negron, Shannon Fox, and Mark Whitmire; DTRA including Rick Fry; DPG including Damon Nicholson, Petr Serguievski, and Allison Hedrick; Chlorine Institute including Therese Cirone and Henry Ward; and the JR II Scientific Advisory Group (SAG) including Leo Stockham, Joe Chang, Steve Hanna, Allison Hedrick, Mike Sohn, and Thomas O. Spicer, III. Special thanks to Michael Donovan for discussions regarding the analysis of the data.

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