Optimization of Gas Generation Testing of Contact-Handled Transuranic Solidified Organic Waste

T. Shokes
North Wind, Inc.
1425 Higham Street, Idaho Falls, ID 83402
United States

K. J. Liekhus
Shaw Environmental, Inc.
9401 Canyon Mesa Drive, Las Vegas, NV 89144
United States

V. Bowman
BBWI
850 Energy Drive, Idaho Falls, ID 83402
United States

E. Schweinsberg
BNG America
850 Energy Drive, Idaho Falls, ID 83402
United States

ABSTRACT

The Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC) requires that drums containing Waste Type IV (solidified organic waste) must be evaluated by gas generation testing (GGT) because a G-value, a measure of gas generation potential, has not been determined for Waste Type IV. Preliminary gas generation testing of Waste Type IV drums at the Advanced Mixed Waste Treatment Project (AMWTP) resulted in a subset of drums exceeding one or both rate limits. This is not an unreasonable phenomenon, given the quantity of source material for hydrogen gas and potentially high concentration of volatile organic compounds (VOCs) in drums containing this waste type. Typically, waste drums in which the flammable gas and total gas generation rates from GGT exceed allowable limits cannot be shipped until these rates are reduced to an allowable level through treatment or repackaging. However, since the gas generation rates are not measured directly, but calculated using test data measurements, there is the possibility that the calculated rates are inaccurate or overly conservative as a result of gas sampling methodology or inaccuracies in equations and assumptions used to estimate total gas release or hydrogen gas generation rates in the GGT system.

In an effort to increase the number of drums that comply with the gas generation rate limits, the Gas Generation Test Program (GGTP) was reviewed at the AMWTP. The objective of the effort

was to identify overly conservative aspects of the GGTP and reduce the level of conservatism by using more realistic parameters and assumptions. In addition, the impact of transportation initiatives in the CH-TRAMPAC, Revision 2 on the number of drums that must undergo GGT and shippability is examined. Based on the presented case study, an optimal payload assembly is recommended for the total gas generation rate and flammable gas generation for Waste Type IV drums.

INTRODUCTION

The Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC) details the transportation requirements for contact-handled (CH) transuranic (TRU) waste in the TRUPACT-II or HalfPACT shipping packages [1]. This paper discusses one of the methods by which U.S. Department of Energy sites may comply with the gas generation requirements of the CH-TRAMPAC, gas generation testing (GGT). The flammable gas requirement states that hydrogen must be limited to be no more than 5 percent by volume in the innermost confinement layer. The drums placed in the shipping packages must be controlled such that the total gases generated in the inner containment vessel (ICV) of the shipping package maintain the inner pressure below the design pressure of the ICV. Compliance with these requirements is met when the flammable gas and/or total gas generation rates of a waste drum are less than or equal to the respective limits. Waste drums are tested until "the rates are shown to be constant or decrease or until the testing period… equals or exceeds the time of the allowed shipping period."[1]

GGT may be performed on CH-TRU waste drums that exceeds the analytical decay heat limit and/or have more than 500 ppm total flammable volatile organic compounds (VOCs). GGT is the required method of compliance for waste that does not have a bounding G value, gas generation potential. Solidified organic waste, Waste Type IV, has an unknown G value and must undergo GGT to demonstrate compliance with CH-TRAMPAC gas generation requirements. During GGT, measurements are taken to determine representative flammable gas and/or total gas generation rates.

A process is described that optimizes each step from performing GGT to determining the payload assembly. Input values that represent the actual system are the best approach to using the model rather than overly conservative assumptions. The sensitivity of parameter values in the model developed at the Advanced Mixed Waste Treatment Project (AMWTP) is presented, as well as comparison of the resulting rates to limits for regulatory compliance. Transportation initiatives for reduced GGT by determining a bounding rate are evaluated for feasibility. Shipping scenarios and the need to make changes to the drums' packaging configurations are discussed, as well as the benefits received in increasing the number of shippable drums and final drum disposition at the Waste Isolation Pilot Plant (WIPP).

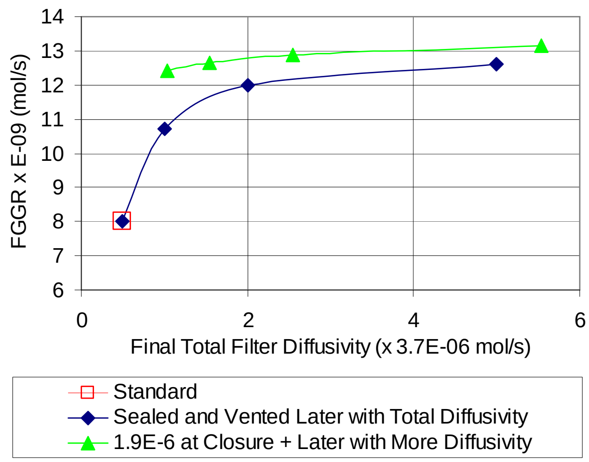
MODELING AND MEASUREMENTS

Sensitivity Analysis

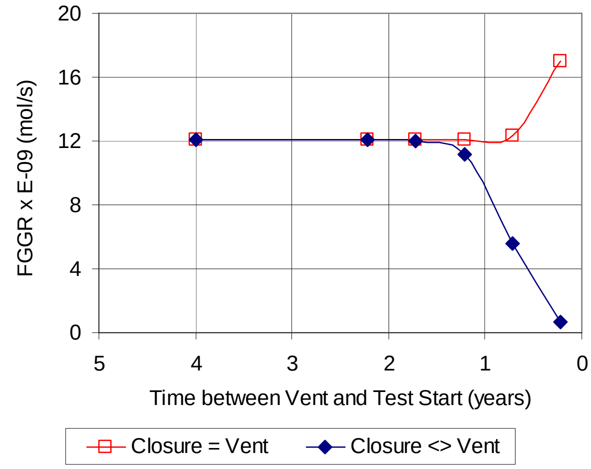
The model at the AMWTP was reviewed to evaluate the possibility of less conservative assumptions or other modifications that would yield a more accurate rate calculation. The standard approach for testing a drum consisted of loading the drum into the canister, heating the unit for at least three days, and taking measurements at 20-hour intervals. The measurements included taking a sample of the canister gas and measuring the hydrogen concentration and measuring the temperature and pressure inside the unit. When it was time to take another measurement, the process was repeated. After data had been collected, the flammable gas generation rate (FGGR) and total gas generation rates (TGGR) were calculated. To perform the calculation, assumptions were made for parameters, including the total diffusivity of filters in the drum lid, closure date, shipping category, and void volume of the drum. The model was changed to allow input of the actual values for a drum, and the sensitivity of the model to parameter values was analyzed. Figure 1 presents the results of the sensitivity analysis performed on a theoretical drum. Only the values for parameters discussed for each sensitivity analysis were changed.

Typically, the filter(s) in the drum lid is assumed to have a filter diffusivity of 1.9E-06 mol/s/mol fraction. Figure 1a represents this scenario with the "Standard" symbol. The two curves represent different venting and filtering scenarios. The curve labeled "Sealed and Vented Later with Total Diffusivity" assumes the drum is not vented at closure and all filters, if more than one, are installed at one later date, the vent date. For this sensitivity test, the closure and vent date; sample date, temperature, pressure, and concentration; and inner layers of confinement were held constant; only the filter diffusivity between closure and venting and between venting and GGT start was changed. The first data point on this curve matches the standard assumption of only one 1.9E-06 mol/s/mol fraction filter. The curve labeled "1.9E-6 at Closure and Later with More Diffusivity" is modeled assuming a 1.9E-06 filter is installed when the drum is packed. At a later date, the same date as the vent date for the other curve, one or more filters of equivalent or higher diffusivity are installed. As shown by Figure 1a, if the filter diffusivity on the drum lid is greater for a given set of measurements, then the resulting FGGR is greater as well, in this case up to 50-percent greater. The rate is proportional to the total filter diffusivity and the length of time the drum has been vented. If data are not available, then a conservative assumption of the filter diffusivity and vent time should be used.

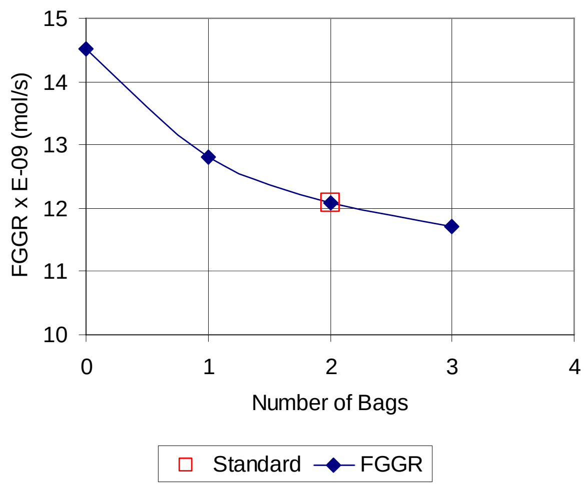
The model is also sensitive to the closure and vent dates of the drum as shown in Figure 1b. All other parameters were held constant. The curve where the closure date equals the vent date shows the effect on the model for the standard assumption used for GGT, i.e., that the drum has not been sealed. To generate the curve where the closure date does not equal the vent date, the time between drum closure and the GGT start date is held constant, approximately 12 years. Only the vent date is changed to show the effect in the model. In this case, no filters are installed in the drum lid between closure and venting, and a 3.7E-06 mol/s/mol fraction filter is installed at the vent date. Based on the results, the calculated FGGR for a given set of measurements will be lower for those drums that are vented, or more filters are installed, close to the GGT start date when the seal time, or time period with lower total diffusivity, is taken into account. This sensitivity analysis also indicates that the diffusivity and vent time may affect the calculated rate. For the case presented here the effect is noticeable beginning about 1.5 years prior to the GGT start date. If it is assumed that the drum is vented at closure, the calculated FGGR increases when the drum is generated close to the GGT start date, in this case about 9 months before the GGT start date.



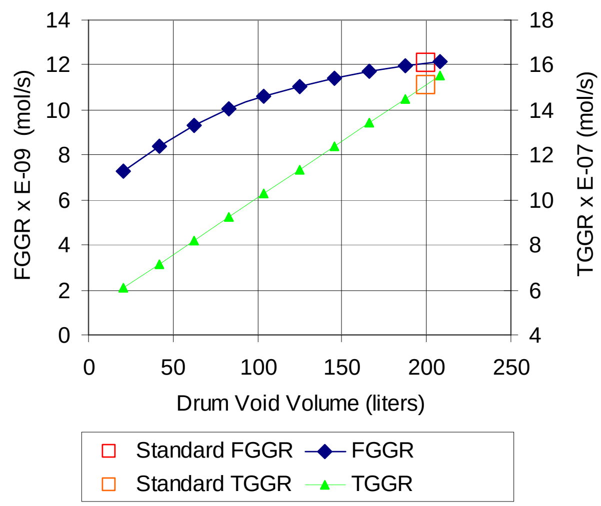
a) Filters in drum lid



b) Closure date



c) Shipping Category (layers of confinement)



d) Void volume

For the GGT model, the assumption inner layers of confinement is typically two liner bags and a 90-mil rigid liner with a hole in the lid of 0.3-inch minimum diameter. The parameter value for layers of confinement for the purposes of the rate calculation is obtained from the shipping category. The sensitivity analysis on the model examines the effect of the bag layers; all other parameter values were held constant. As shown in Figure 1c, the calculated FGGR increases when fewer bag layers are present, approximately a 20-percent increase from two bags to zero bags. Therefore, it is important to select a shipping category that represents the actual layers of confinement in a drum during GGT when performing the rate calculation.

The void volume assumed in the drum is an input value for the FGGR and TGGR calculated rates. The typical void volume assumed for a drum is 200 liters, which is equivalent to a fill factor of about 4-percent. The standard FGGR and TGGR data points in Figure 1d indicate the rates that would result from the standard assumption. To determine the effect of void volume on the calculated rate, the void volume was varied while all other input values were held constant. When the void volume is reduced, both the FGGR and TGGR decrease by approximately 30 and 50 percent, respectively, for void volumes from 208 to 21 liters (fill factors from 0 to 90 percent).

The sensitivity analysis demonstrates the impact on the calculated rates for parameter values that are typically assumed. The net effect of these assumptions would vary from one drum to another just as the actual values vary and, therefore, is unquantifiable. At AMWTP, the model was changed to use the actual values for parameters discussed here. The model uses two dates before the GGT start date: the date the drum was packed and the date of the last filter installation. Based on the total number of filters installed at the time of testing, the total diffusivity is determined assuming all filters have a diffusivity of 3.7E-06 mol/s/mol fraction. If more than one filter is present at the GGT start date, then it is assumed that only one filter is installed at the date of the last filter installation; all other filters are present from the pack date of the drum. Based on the real-time radiography (RTR) or visual examination (VE) of the drum, the shipping category matching the number of bag layers is selected for the GGT model. The fill factor from RTR or VE is also used to estimate the void volume in the drum. These assumptions were developed to more accurately determine the FGGR and TGGR of drums.

Measurements

While reviewing preliminary GGT data at AMWTP, the conditions under which measurements were taken were reviewed. The focus was on when the physical conditions of the test were changed over time. For instance, the temperature and pressure used at each bound condition need to be accurate. The temperature and pressure are recorded each time the hydrogen concentration is measured. The temperature and pressure are also measured when the GGT canister is sealed when GGT starts. These values when GGT starts are used for the FGGR to calculate the initial moles of gas present in the drum and GGT canister at the beginning of the test, i.e., the initial conditions. The GGT canister is also leak tested. Preliminary GGT at AMWTP showed that the TGGR was frequently negative. The process for taking measurements was to take the gas sample from the GGT canister volume and then measure the pressure and temperature. When taking a subsequent measurement, these steps were repeated. Each pair of measurements yielded rates; however, the removal of gas was not accounted for in the subsequent pressure measurement. To verify and quantify the effect of taking the gas sample before measuring the pressure on the TGGR, GGT was performed where the pressure was measured before and after taking the gas sample on the second measurement for 45 drums. For all 45 drums, the TGGR was greater when calculated using the pressure measurement before the gas sample, as expected. Table I presents the range and average change in pressure resulting from taking the gas sample. Preliminary GGT data presented in this report when the second pressure measurement was not taken before the sample is corrected by adding the average pressure difference to the original measurement.

Table I. Statistics on the Change in Pressure Before and After Taking a Gas Sample.

Number of Drums	Pressure Difference (psia)			
	Minimum	Maximum	Average	Standard Deviation
45	0.031	0.544	0.231	0.106

SOFTWARE AND RESULTS

AMWTP has begun implementing the model in software. The software is a Microsoft Access database with forms to provide a graphical user interface. An example input form is shown in Figure 2. The software maintains an electronic record of each GGT test and all measurements. Operators can enter the data directly into the software and, if necessary, return to correct data entry errors or add more data as measurements are collected. The software calculates the FGGR and TGGR between each pair of valid measurements. Checks are in place to verify that each pair of samples are at least 20 hours apart, Waste Type IV undergoes elevated temperature testing, and hydrogen and methane concentrations are provided from headspace gas analysis for Waste Type IV. The headspace gas concentrations of hydrogen and methane are used to calculate the FGGR using theoretical analysis [2]. The CH-TRAMPAC requires that the GGT "rates are shown to be constant or decrease or until the testing period… equals or exceeds the time of the allowed shipping period" [1]. The GGT software determines whether the FGGR and TGGR are constant and decreasing. If the rates are constant or decreasing the output summary report for the drum's test includes text that the test may be stopped (Figure 3). If the rates are increasing, then the summary indicates to continue testing. The software assists operators and others with ascertaining if the test is compliant with regulatory requirements. The central location for all GGT data facilitates reviews of data trends with other values such as flammable volatile organic compounds (VOCs) or GGT process improvements.

The AMWTP software was used to calculate rates using the AMWTP model based on preliminary GGT tests. If the fill factor was not available, the rates were calculated using the standard drum void volume assumption. For Waste Type IV tests, if hydrogen and methane headspace gas data were not available, the maximum ratio was used based on available data. GGT data was collected under Revision 19 of the TRUPACT-II Authorized Methods of Payload Control and included Waste Type I and IV. The data for each pair of measurements on a drum were re-evaluated using the AMWTP model, and the rates were compared to the limits: the maximum allowable flammable gas generation rate (AFGGR), assuming the total concentration of flammable VOCs is less than or equal to 500 ppm, and the maximum allowable total gas release rate, if applicable. For Waste Type I, 169 drums were tested and 96% passed the AFGGR. For Waste Type IV, 69% of the drums passed the AFGGR and the maximum allowable total gas release rate. Although the information about the number of drums passing the limits is interesting, the intent of GGT is to establish a constant or decreasing rate. Out of the 12 drums with data available for this assessment, three drums qualified to stop the test, i.e., a constant or decreasing rate(s) had been determined.

Flammable VOC data were available for 96 drums. The total concentration of flammable VOCs was calculated for each drum. Zero was used for non-detectable analyses. Table II presents some statistical values on the total concentration of flammable VOCs, which has a range of about 10,000 ppm. However, approximately half the drums had a total concentration less than or equal to 500 ppm. The 95% upper confidence limit of the 95th percentile (95UTL) was determined for an upper bound using the non-parametric statistical technique of bootstrapping[1]. This methodology was chosen to be consistent with the long-term objective procedure of the Unified Flammable Gas Test Procedure of the CH-TRAMPAC.[1]

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[1] Note: Bootstrapping is a method for estimating the distribution by resampling with replacement from the original set of samples.[3]

Table II. Range, Mean, and Upper Bound for the Total Concentration of Flammable VOCs.

Waste Type	Total Concentration of Flammable VOCs (ppm)			
	Minimum	Maximum	Mean	95UTL
I	2.3	13,000	4,700	12,000
IV	14	10,000	700	10,000

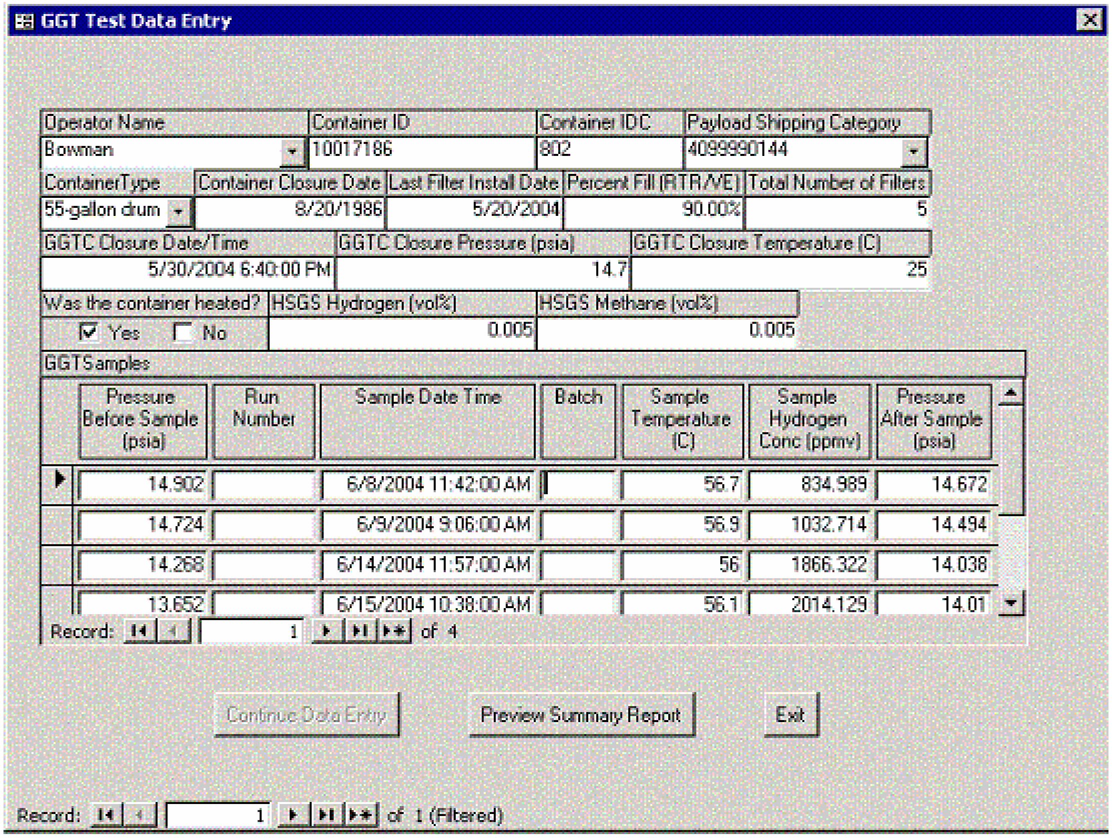


Fig. 2. Example input form from GGT software.

The relationship between the measured values was also examined as shown in Figure 4. Figure 4a includes 57 Waste Type I and 41 Waste Type IV drums and shows the FGGR versus the total concentration of flammable VOCs. Most of the Waste Type IV data points occur between 0 and 1,000 ppm. Based on the information presented here, a clear trend between the FGGR and VOCs does not exist. Figure 4b shows the FGGR versus the TGGR. The FGGR tends to accumulate about a TGGR of zero. For the TGGR to remain about zero for any FGGR, one or more mechanisms are removing/consuming gas from the void volume of the drum and GGTC.

PRODUCTION

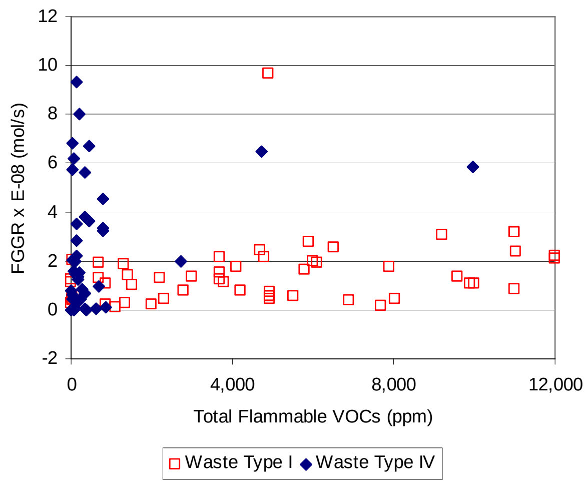
The time it takes to perform GGT sets it apart from other characterization methods. Table III presents the typical time to perform the steps of GGT, which result in a total of 14 days to test a drum one time. Sites that perform GGT typically have many GGT canisters so they can perform GGT on many drums at one time. Historically, AMWTP has had 40 GGT canisters available for testing, resulting in a maximum testing capacity of 80 drums per month. AMWTP has a current inventory of approximately 10,000 Waste Type IV containers, 9,000 of which are 55-gallon drums. Based on the estimated inventory, the time of testing completion is mid-2016 unless the testing capacity is increased and/or a technology or regulatory initiative is used to reduce the number of drums being tested.

Gas Generation Test Summary Data Sheet

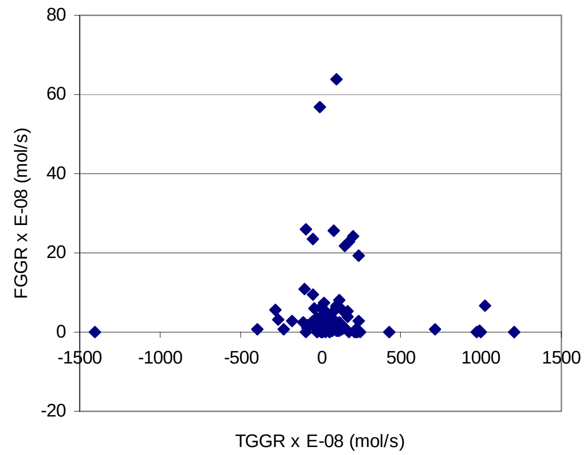
Operator Name:	Bowman
Container ID:	10017186
Container IDC:	802
Payload Shipping Category:	4099990144
ContainerType:	55-gallon drum
Container Closure Date:	8/20/1986
Container Vent Date:	5/20/2004
Total Number of Filters:	5
Percent Fill (RTR/VE):	90.00%
GGTC Closure Date/Time:	5/30/2004 6:40:00 PM
GGTC Closure Pressure (psia):	14.7
GGTC Closure Temperature (C):	25
Initial Batch:	
Initial Sample Date/Time:	6/14/2004 11:57:00 AM
Initial Sample Pressure (psia):	14.038
Initial Sample Temperature (C):	56
Initial Sample Hydrogen Concentration (ppmv):	1866.322
Final Batch:	
Final Sample Date/Time:	6/15/2004 10:38:00 AM
Final Sample Pressure (psia):	13.652
Final Sample Temperature (C):	56.1
Final Sample Hydrogen Concentration (ppmv):	2014.129
Container heated during test:	☑
HSGS Hydrogen (vol%):	0.005
HSGS Methane (vol%):	0.005
Test Duration (hr):	376
Flammable Gas Generation Rate (mol/s):	3.255E-08 — Previous FGGR (mol/s): 3.376E-08
Total Gas Generation Rate (mol/s):	-2.657E-06 — Previous TGGR (mol/s): -2.345E-07
TestStatus:	Stop Test

Initial Data Entry By: ____________________

Fig. 3. Summary output report for a drum test from GGT software



a) FGGR versus total flammable VOCs



b) FGGR and TGGR for Waste Type IV

Fig. 4. Plots of relationships between flammable VOCs and concentrations and rates.

Table III. Typical Durations for Steps in GGT.

Step	Process Step	Duration	Comment
1	Set up	1 day	Includes lead test
2	Heating & Stability check	8 days	Activity is to check values via walk round, approx. 20 minutes once every 2 hours
3	Test	4 days	Multiple samples taken in 20 hour or greater intervals to demonstrate steady rates or test for the shipping period (10-day only)
4	Cool	(½ - 1 day)	Typical duration preferable if left overnight. Some overlap with activities 3 and 5
5	Dispatch	1 day	Activities 1 and 5 are typically performed together.
	TOTAL	14 Days	

Reduced Testing

The UFGTP Long-Term Objective Implementation Methodology in the CH-TRAMPAC provides a methodology for reduced GGT [4]. The implementation methodology described how to determine an upper bounding rate, the 95UTL, for a subpopulation of drums. The 95UTL for the rates is used to replace test results for untested drums in the same population. The methodology consists of the following steps:

- Establishment of a population of drums
- Random selection of drums for GGT
- Performing GGT and determine the FGGR and TGGR
- Determining the 95UTL of the FGGR and TGGR using a non-parametric technique
- Application of the 95 UTL rates to the untested drums in the population.

This initiative was applied only to the limited data set available for Waste Type IV drums discussed in this report for the purposes of demonstration. Although Waste Type I drums were tested, these drums can undergo the CH-TRAMPAC, Revision 2, flammability assessment with decay heat or headspace gas measurement; GGT is not required.

The populations to examine the feasibility of using this methodology at AMWTP were established by Waste Type and item description code (IDC). Ninety-nine Waste Type IV drums have GGT data. The IDCs and number of drums for each IDC are listed in Table IV. The number of GGT drums does not meet the minimum required subpopulation size, and sampling more drums may yield different results than the subsequent analysis performed for demonstration only. Ten is the required number of samples to perform bootstrapping; therefore, IDCs 422, 700, and 823 are excluded as populations. As shown by the minimum required subpopulation size, it is beneficial to establish populations as large as is feasible to minimize the number of drums that undergo GGT. However, practical limitations, such as storage space and maintaining shipments to the WIPP, may exist that deter the establishment of large populations.

Table IV. Number of Drums for Each Waste Type IV and IDC.[a]

IDC/ Waste Type	Number of GGT Drums	Total Population (estimate)	Minimum Required Subpopulation Size	Comments
003	53	9,077	264	
422	1	-	-	Invalid sample size for bootstrapping
700	5	-	-	Invalid sample size for bootstrapping
801	24	828	205	
802	15	199	115	
823	1	-	-	Invalid sample size for bootstrapping
Waste Type IV	99 (total)	10,164	264	

[a] The drums with GGT data were not randomly selected from the population. The required subpopulation must be randomly selected from the total population for the Long-Term Objective Implementation Methodology results to be valid.

Table V presents the 95UTL that was determined for the FGGR and TGGR for populations that have an adequate number of drums to perform the bootstrapping. The 95UTLs will enable a preliminary analysis on potential application of the methodology. Additionally, the drums were not randomly selected from the population. The CH-TRAMPAC states "containers selected for evaluation… must be representative of the population with random or stratified sampling techniques used to avoid any bias in container selection." If drums are not randomly selected, then it must be clearly shown that the results are not biased, or if the results are biased, then it must be clearly shown to be biased in a conservative direction, i.e., high 95UTL. If a drum is randomly selected that has been tested, the GGT results may be used and retesting is not required.

The FGGR 95UTL was compare to the AFGGR for each drum based the shipping category used during GGT and assuming that the total concentration of flammable VOCs is less than or equal to 500 ppm. All shipping categories assigned during testing assume a 60-day shipping period with a full payload (14 drums) in the TRUPACT-II. All FGGR 95UTLs were greater than the AFGGR for any packaging configuration. The packaging configuration with the highest limit consisted of zero bag layers, a rigid liner with a 0.3-inch diameter hole, and a 3.7E-06 mol/s/mol fraction diffusivity filter in the drum lid. The TGGR 95UTL was compared to the maximum allowable total gas release rate from Table 5.2-11 of the CH-TRAMPAC [1]. The TGGR 95UTL for each population was greater than the allowable total gas release rate. The 95UTLs are ineffective if shipping is achieved with a 60-day shipping period and a full payload. The evaluation continues by assessing the effect of payload assembly initiatives for TGGR and FGGR from the CH-TRAMPAC on the shippability of these populations.

Table V. The 95UTL for Each IDC and Waste Type Population.

Rate	IDC/ Waste Type	95UTL (mol/s)	Rate Limit (mol/s) [a]	95UTL ≤ Rate Limit
FGGR	003	5.9E-07	Based on Shipping Category Assume 60-day, full payload	No, for all shipping categories
	801	6.7E-08		No, for all shipping categories
	802	6.8E-08		No, for all shipping categories
	IV	2.3E-07		No, for all shipping categories
TGGR	003	9.8E-06	3.97E-06	No
	801	1.2E-05		No
	802	1.0E-05		No
	IV	1.0E-05		No

[a] See Chapter 5 of Reference 1.

Total Gas Generation Rate

The initiative for the TGGR allows credit for dunnage drums in a payload assembly. It also allows for mixing with different Waste Types that may have lower rates. For this assessment, only the Waste Type IV drums will be assessed, and all drums in the payload assembly will be assumed to be from the Waste Type IV population. The initiative consists of calculating the payload TGGR and the payload TGGR limit taking credit for dunnage. (The CH-TRAMPAC total gas release rate is called the TGGR in this paper.) Only payload assemblies of 55-gallon drums in either the TRUPACT-II or HalfPACT are evaluated.

Application of this initiative to the Waste Type IV TGGR 95UTL yields the results presented in Table VI. As shown in Table VI, the payload assembly with the most number of generators in the TRUPACT-II has eight drums. The payload assembly in the HalfPACT is compliant with the payload TGGR limit with a payload of five drums. Based on these results, the Waste Type IV population meets the TGGR requirements when assembled as seven waste drums in the TRUPACT-II or 5 drums with two dunnage in the HalfPACT.

Table VI. Compliance Assessment for TGGR for Payload Assemblies with Dunnage in the TRUPACT-II and HalfPACT.

Number of Generators	Number of Dunnage Drums	Payload TGGR (mol/s)	Payload TGGR Limit (mol/s)	Compliant
TRUPACT-II				
14	0	1.4E-04	5.54E-05	Fail
9	5	9.0E-05	7.89E-05	Fail
8	6	8.0E-05	8.36E-05	Pass
7	7	7.0E-05	8.83E-05	Pass
HalfPACT				
7	0	7.0E-05	4.17E-05	Fail
6	1	6.0E-05	4.64E-05	Fail
5	2	5.0E-05	5.11E-05	Pass

Flammable Gas Generation Rate

For the FGGR, shipping period and drum packaging configuration contribute to the shippability of a payload assembly. All waste drums in the payload assembly are assumed to each have the same shipping category and a total flammable VOC concentration less than or equal to 500 ppm. Given these assumptions and that the FGGR is the same for each drum in the payload assembly(the FGGR 95UTL), an evaluation of the packaging configuration was performed by calculating the maximum resistance to hydrogen release of the packaging configuration, multiplied by 10^{-4}, or the last four digits of the shipping category (ZZZZ) [5]. Equation 1 calculates the ZZZZ portion of the shipping category by rearranging the equation for AFGGR (also referred to as CG in the CH-TRAMPAC) and substituting the FGGR 95UTL for the AFGGR.[1]

$$\text{ZZZZ} = \text{rounddown}\left(\frac{0.05}{10{,}000 \times \text{FGGR95UTL}}\right) \qquad \text{(Eq. 1)}$$

Evaluating the calculation for Waste Type IV yields 0021 for the maximum acceptable ZZZZ. Proceeding onto to reviewing the components of ZZZZ by referring to the Numeric Payload Shipping Category Worksheet in the CH-TRU Payload Appendices [5], The total resistance factor sum must be less than or equal to 2,100. This value is a sum of resistance factors that includes the load type (payload assembly configuration and shipping period), payload container lid filter, rigid liner, and plastic bag layers, typically liner bags for organic sludge waste.
Table VII presents the evaluation of some of the confinement layers, filters, and shipping periods that may be in ZZZZ. Either a liner bag or 55-gallon drum with a 3.7E-06 mol/s filter would result in the use of a resistance factor that alone would exceed the maximum acceptable ZZZZ.

Table VII. Evaluation of Layers of Confinement and Shipping Periods for Maximum Acceptable ZZZZ.

Layer of Confinement/Load Type	Resistance Factor [a]	Acceptable
Twist and Tape Liner Bag	2142	No
Rigid Liner with 0.3-inch diameter hole	197	Yes
55-gallon drum 3.7E-06 filter	2703	No
55-gallon drum 18.5E-06 filter	541	Yes
Load Type: 10-day controlled shipment, 14 55-gallon drum	1192	Yes
Load Type: 10-day controlled shipment, 7 55-gallon drums	374	Yes

[a] The resistance factors were obtained from the Numeric Payload Shipping Category Worksheet in the CH-TRU Payload Appendices [5] except for the load type for a 10-day controlled shipment with seven 55-gallon drums. This load type includes seven dunnage drums and was calculated using the mixing of shipping category methodology.[5]

ZZZZs with the acceptable shipping category components are shown in Table VIII. The ZZZZ was calculated for each payload configuration for drums with and without a rigid liner. For drums that already exist with zero bag layers, the drum need not be opened to remove the liner lid. For drums with liner bags, the drum would be opened to slash the bags, rendering them innocuous as layers of confinement. During this process, the rigid liner lid should also be removed.

Table VIII. ZZZZ with Acceptable Shipping Category Components.

	10-day Controlled Shipment			
	14 drums	14 drums	7 drums	7 drums
Rigid Liner with 0.3-inch diameter hole	197		197	
55-gallon drum 18.5E-06 filter	541	541	541	541
Load Type	1192	1192	374	374
ZZZZ	0020	0018	0012	0010

Within the FGGR limit equation, the 0.05 constant is the allowable flammable gas concentration (0.05 mol fraction) in the innermost confinement layer when drums have less than or equal to 500 ppm total flammable VOCs. When drums have greater than 500 ppm flammable VOCs, the analysis with the UFGTP uses the Mixture Lower Explosive Limit methodology (MLEL) [1] to account for the presence of these flammable VOCs in the drum which reduces the 0.05 maximum allowable flammable gas concentration. Rearranging Equation 1 to solve for the equivalent flammable gas concentration for the FGGR 95UTL yields Equation 2.

$$EqFGC = 10{,}000 \times FGGR95UTL \times ZZZZ \quad \text{(Eq. 2)}$$

After determining the equivalent flammable gas concentration, an estimate of the maximum concentration of flammable VOCs measured in the headspace gas sample was estimated as shown in Table IX using the MLEL methodology in the CH-TRAMPAC. This analysis assumes that the shipping category used during shipping is for a 55-gallon drum with a filter of 18.5E-06 mol/s/mol fraction diffusivity, rigid liner with 0.3-inch diameter hole, and zero bag layers. Two VOCs, one with the least and one with the greatest contribution to flammability, were used to estimate the range for the maximum allowable total VOC concentration in the headspace gas of the drum. The results indicate the benefit by a factor of about three in the allowable flammable VOC concentration by shipping the Waste Type IV containers in payload assemblies of seven waste drums. Out of 39 Waste Type IV drums with flammable VOC data available, seven drums had a total flammable VOC concentration greater than 500 ppm. The maximum total flammable VOC concentration was less than 10,000 ppm.

Table IX. Estimate of the Best and Worst Case Upper Bound on the Total Flammable VOC Concentration in Waste Type IV Drums.

ZZZZ	Number of Generators	EqFGC (ppm)	Total Flammable VOC (ppm)	
			Worst Case	Best Case
0020	14 drums	46,000	≤ 500	3,200
0018		41,400	540	6,900
0012	7 drums	27,600	1,400	18,000
0010		23,000	1,700	21,700

CONCLUSION

The demonstration of an approach to optimize GGT yielded more accurate gas generation rates, reduced the number of drums that must undergo GGT, and increased the efficiency of establishing shipping configurations. The optimization approach consisted of reviewing the GGT program from the foundation of GGT, the model and assumptions, through to the possible packaging configurations and payload assemblies for shipping the drums to WIPP. By reviewing multiple aspects of the GGT program and shippability, the cumulative effect yields an increased GGT processing rate for drums and global decisions for shippability.

The demonstration presented was based on the limited data set and preliminary analysis. Additional GGT will be performed to meet the minimum number of required samples for the Long-Term Objective Implementation Methodology, and lack of bias will be clearly shown for the 95UTL results. However, some conditions were identified that may increase shippability.

- Use the 10-day controlled shipment.
- Build payload assemblies of one 7-pack in the TRUPACT-II.
- Breach all plastic bag layers.
- Install one or more filters in the drum lid such that the total diffusivity is greater than or equal to 18.5E-06 mol/s/mol fraction.

The benefits of a payload assembly of seven waste drums for WIPP include placing full 7-packs in the WIPP repository, which results in a total of 21 drums in the stack. The 7-pack of dunnage in the TRUPACT-II will not be placed in the WIPP repository. All other payload assembly options would emplace fewer than 21 drums. The only way to place more waste in the footprint of a 7-pack is to use machine compaction, a process that cannot be applied to Waste Type IV. In summary, the optimization process accomplishes the following benefits:

- An FGGR and TGGR more closely approaching the real rate.
- Successful application of the UFGTP Long-Term Objective Implementation Methodology reducing the number of drums for GGT.
- Determining the optimal payload assembly, shipping period, and packaging configuration.
- The payload assembly of seven waste drums may also include some drums with total flammable VOCs greater than 500 ppm.
- Efficient disposition of the waste drums in the WIPP.

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