

## **ANALYSIS AND TESTING OF THE METAL PARTS FURNACE FOR THE DEMILITARIZATION OF CHEMICAL WARFARE MUNITIONS**

RONALD L. FOURNIER\*

*Department of Chemical Engineering, The University of Toledo, Toledo, OH 43606 (U.S.A.)*

DEANE A. HORNE, FRANKLIN G. RINKER

*Maumee Research and Engineering, Inc., Perrysburg, OH 43551 (U.S.A.)*

and

KERM JACKSON

*CAMDS, Tooele Army Depot, Tooele, UT 84074 (U.S.A.)*

(Received April 1, 1989; accepted in revised form August 20, 1989)

### **Summary**

Chemical munitions probably contain the most toxic materials ever created by man and represent a unique challenge for those involved in their destruction. Prototype testing of the thermal destruction processes for chemical munitions has been carried out at the Chemical Agent Munitions Disposal System (CAMDS) located at Tooele Army Depot, Utah.

The munition metal parts containing up to 5% residual agent are thermally decontaminated in a roller hearth type furnace, the Metal Parts Furnace (MPF). The drained munitions are heated to a temperature of at least 1000 °F for at least 15 minutes to insure complete destruction of any remaining agent residue. During this heating process the residual agent will vaporize. The vaporized agent burns within the MPF and the MPF afterburner prior to treatment of the combustion product gases in the pollution abatement system. Agent vaporization is a rapid unsteady process with peak Btu loadings on the MPF furnace as high as 10 million Btu/h. Furthermore there are 14 different munition types containing 3 different types of chemical agents. These range from a load of 96 105-mm projectiles containing as little as 0.08 lbs of the nerve agent GB per projectile to a ton container with 80 lbs of the nerve agent VX. Clearly the control system of the MPF system must be flexible enough to handle such a wide variety of thermal loads.

To evaluate and predict the performance of the MPF, tests have been performed at CAMDS by using a variety of munitions containing chemical agent simulants. The simulants were selected on the basis of comparable boiling points, heat of vaporization, and heat of combustion. A mathematical model of the MPF has been developed to predict the heating rate of the munition and the vaporization rate profiles of the agents and their simulants. The results of the model have been compared to simulant testing in ton containers at CAMDS. The results show good agreement with the mathematical model predictions.

---

\*Author to whom correspondence should be addressed.

## 1. Background

The United States has a large quantity of chemical warfare (CW) munitions stored at eight U.S. Army installations within the United States and on Johnston Island, located 717 nautical miles west southwest of Honolulu, Hawaii. Munition types that make up this country's CW stockpile include bombs, rockets, land mines, spray tanks, cartridges, projectiles, and bulk containers. Table 1 briefly describes the munitions in the CW stockpile.

The munitions and bulk items that comprise the U.S. CW munition stockpile are filled with one of the following lethal chemical agents: the nerve agents GB or VX, and the blister agent mustard [1]. These chemical agents are liquids at room temperature. The nerve agents are organic esters of substituted

TABLE 1

### U.S. Chemical Warfare Munitions

Type	Description	Fill	Explosives	Propellant	Fuse
M55 <sup>a</sup>	115 mm Rocket	10.7 lb GB or 10.21 lb VX	3.2 lb	19.31 lb	yes
M23 <sup>a</sup>	Land mine	10.5 lb VX	0.90 lb	none	yes
M2/M2A1	4.2" Mortar <sup>b</sup>	6.0 lb H/HD	0.14 lb	0.6 lb	yes
M60	105 mm cartridge <sup>b</sup>	3.0 lb H/HD	0.26 lb	2.8 lb	yes
M360	105 mm cartridge <sup>b</sup>	1.6 lb GB	1.1 lb	2.8 lb	yes
M110	155 mm projectile	11.7 lb H/HD	0.83 lb	none	no
M104	155 mm projectile	11.7 lb HD	0.83 lb	none	no
M121A1	155 mm projectile	6.5 lb GB or VX	2.45 lb	none	no
M122A1	155 mm projectile	6.5 lb GB	2.45 lb	none	no
M426	8" projectile	14.5 lb GB or VX	7.0 lb	none	no
MC-1	750 lb bomb	220 lb GB	none	none	no
MK-94	500 lb bomb	108 lb GB	none	none	no
TC	ton container	1600 lb GB, VX, or HD	none	none	no
TMU-28	spray tank	1356 lb VX	none	none	no

<sup>a</sup>Not processed in the MPF.

<sup>b</sup>A projectile, burster, fuse, cartridge casing, propellant, and primer comprise a cartridge.

phosphoric acid. Nerve agents affect body functions by inhibiting cholinesterase enzymes leading to accumulation of acetylcholine and subsequent paralysis. GB is more volatile than VX and is readily absorbed into the body by inhalation, ingestion, and through the skin and eyes. VX is absorbed into the body primarily through skin penetration. The toxicity of VX is 3–10 times that of GB. Exposure to either agent can result in death within minutes.

Blister agents are local irritants and systemic poisons attacking the eyes, lungs, and blistering the skin with either liquid or vapor contact. Symptoms of exposure usually do not appear for several hours. Mustard blister agents include Levinstein mustard (H) and distilled mustard (HD). Table 2 [1] provides a summary of the physical and chemical properties of the CW agents.

The country's stockpile of CW munitions is aging being 19–33 years old. In 1986 the U.S. Congress mandated that the military stockpile (less 10%) be destroyed as part of a modernization effort for the entire U.S. chemical warfare capability. The disposal of these CW munitions presents a unique challenge, since these items may contain both an extremely toxic fill (the chemical agent)

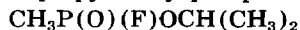
TABLE 2

Physical properties of CW agents

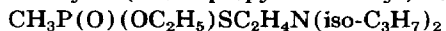
Agent Name	GB	VX	HD
Common name	Sarin	—	Distilled mustard
Mol. Wt.	140.1	267.4	159.1
Liquid density (25°C)	1.089	1.0083	1.27
Freezing Pt. (°C)	–56	–39	14
Boiling Pt. (°C)	158	298	217
Vapor pressure at 25°C (mmHg)	2.9	0.0007	0.072
Heat of vaporization (Btu/lb)	144.0	141.0	169.0
Flash point (°F)	—	318	221
Heat of combustion (Btu/lb-HHV)	8710	13150	7340
Liquid specific heat (Btu/lb°F)	0.416	0.484	0.333
Vapor density (relative to air)	4.86	9.2	5.5
Decomposition temp. (°C)	400–500	700–800	149–177
LD <sub>50</sub> (mg min/m <sup>3</sup> )	100 (respiratory)	100 (skin)	1500 (respiratory)

*Chemical Name and Formula*

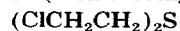
GB isopropylmethyl phosphonofluoridate



VX O-ethyl-5-(2-diisopropylaminoethyl)methyl phosphonothiolate



HD bis(2-chloroethyl)sulfide



as well as energetic materials such as explosives and propellants. The special hazards associated with chemical demilitarization operations require considerable safeguards in order to dispose of this material in a safe and environmentally acceptable manner. In response to these requirements, the U.S. Army has developed methods and procedures on the leading edge of technology for hazardous waste disposal.

The first full-scale demilitarization facility, called the Johnston Atoll Chemical Agent Disposal System (JACADS), is currently under construction on Johnston Island [2]. To support the development of the process design for JACADS, the U.S. Army initiated, in 1982, a comprehensive testing program at the prototype facility, the Chemical Agent Munitions Disposal System (CAMDS) located at Tooele Army Depot, Utah. This \$67 million facility first became operational in September 1979 and serves as a test facility to evaluate various processing operations for possible incorporation into future large-scale demilitarization facilities such as JACADS. In addition to JACADS, 8 additional plants similar to the JACADS facility are being planned to dispose of the CW munitions located within the Continental United States.

Destruction of the chemical munitions is based on incineration of the munition components. Generically, all munition types fall into one of three categories: rockets and mines, projectiles and cartridges, and bulk items. For all three munition categories, the demilitarization process involves two distinct operations: preparation of the munition for thermal treatment, followed by thermal processing. Munition preparation is accomplished by using specially designed machines for removing explosive components by reversing the assembly process, for shearing rockets and explosives, and for draining the agent from the munitions. The thermal destruction operations which form the heart of the demilitarization process are based on four furnaces: the Liquid Incinerator System (LIC), the Deactivation Furnace System (DFS), the Metal Parts Furnace System (MPF), and the Dunnage Incinerator System (DUN). The incinerators have been designed for compliance with applicable RCRA and Clean Air Act requirements.

The LIC processes the bulk of the chemical agent drained from the munitions. The LIC is a two-chamber, air-atomized, liquid injection incinerator. M55 rockets and M23 land mines, as well as the other munitions' explosive and propellant components are processed in the DFS rotary kiln. Metal parts which have been in contact with liquid agent are thermally decontaminated in the roller hearth metal parts furnace (MPF). In addition to the decontamination of the metal parts, this furnace is also designed to incinerate a residual agent "heel" of up to 5% by weight of the agent fill of each munition. The DUN is designed to process dunnage including agent contaminated wood, wooden pallets impregnated with preservatives, contaminated protective clothing, and other packaging materials. Each furnace system has an independent pollution

abatement system designed to scrub the products of combustion. The primary products of combustion are shown in Table 3.

With this background on chemical munitions demilitarization, the focus of the effort described in this paper is on understanding the dynamic effects which occur when processing chemical munitions in the metal parts furnace. Figure 1 illustrates the basic design of the MPF. The JACADS MPF is a three zone furnace. The first zone is the heat up zone, the second is the vaporization zone, and the final zone is the 5X zone. The 5X criterion insures complete decontamination of the metal parts. This criterion requires that the munition metal parts be maintained at a temperature of at least 1000°F (~530°C) for at least 15 minutes. For bulk items as an example, the munition spends 35 minutes in each zone with the zone temperatures respectively 1150, 1200 and 1400°F.

Agent vaporization of the residual 5% heel of the chemical agent is a rapid unsteady process with peak Btu loadings on the MPF system as high as 10 million Btu/h. Furthermore as shown earlier in Table 1, there are 14 different types of munitions containing 3 different types of chemical agents. The design and control of the MPF system will therefore require an understanding of the timing of the onset of agent vaporization, the duration of the agent vaporization process, as well as the peak vaporization rate for each agent-munition combination.

A unique problem for chemical agents is the inability, because of their extreme toxicity, to do extensive prototype testing of the various agent-munition combinations. The approach described in this paper to understand the agent vaporization process was to identify and to use as agent simulants, common industrial compounds which match as closely as possible the pertinent thermal properties of the actual chemical agents. Proper selection of the agent simulants is based in part on the use of a mathematical model of the munition heating and vaporization processes which occur within the MPF. The MPF model allows for comparison of the vaporization rate of the actual agent with its simulant for various munition types under a variety of MPF operating scenarios. Preoperational tests using the agent simulants along with calibration of the mathematical model will then minimize uncertainty and ensure safe furnace operation when the actual agent munitions are processed.

TABLE 3

Agent products of combustion

Agent	Products of combustion
GB	CO <sub>2</sub> , H <sub>2</sub> O, P <sub>2</sub> O <sub>5</sub> , HF, NO <sub>x</sub>
VX	NO <sub>x</sub> , P <sub>2</sub> O <sub>5</sub> , SO <sub>2</sub> , CO <sub>2</sub> , H <sub>2</sub> O
HD	CO <sub>2</sub> , SO <sub>2</sub> , HCl, H <sub>2</sub> O, NO <sub>x</sub>

Recommended Thermocouple Locations  
with Ton Containers in Place

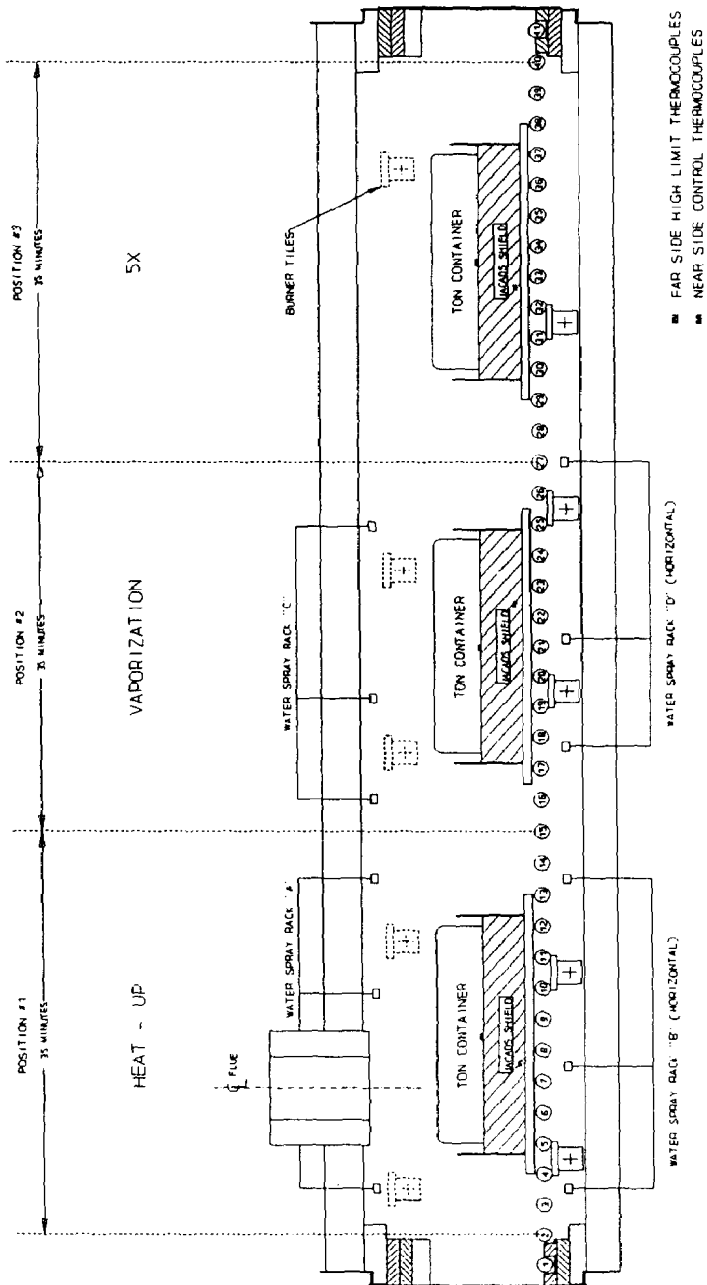


Fig. 1. JACADS metal parts furnace cross section.

## 2. Simulant selection

A search was conducted to find common industrial compounds to use as simulants for the chemical agents. An ideal simulant would provide a close match of all of the physical properties of the agent. Unfortunately there is no ideal simulant. Certain properties must be compromised. Therefore, the physical properties which should be matched are those which are important in modeling the agent vaporization process which occurs in the metal parts furnace. Generally the process of destroying agents thermally involves vaporizing the residual agent, then combusting the vapors either in the furnace or in the primary fume burner. The process events which a simulant needs to reproduce are the time at which vaporization starts and the peak vaporization rate. The physical properties which control these events are the boiling point, the heat of vaporization, and the heat of combustion. The boiling point controls the timing of vaporization, and the heat of vaporization controls the vaporization rate. The heat of combustion provides the Btu loading to the furnace or fume burner. Additional criteria for suitable simulants are that they are safe to use, assuming reasonable care is taken to limit exposure of personnel, and that they are reasonably inexpensive. Table 4 lists a number of simulants and agents with their physical properties.

To illustrate the selection of a simulant consider propylene glycol, which in the past has been used as a simulant for GB. Propylene glycol fits the safety and cost constraints, it is nontoxic and relatively inexpensive. Its heat of combustion is close to that of GB, but its boiling point is about 50°F (28°C) higher, and more importantly, its heat of vaporization is more than twice that of GB. Therefore, propylene glycol will start vaporizing later (higher boiling point),

TABLE 4

Agent and simulant physical properties

Compound	Heat of vaporization (Btu/lb)	Heat of combustion (Btu/lb)	Boiling point (°F)
<i>Simulants</i>			
Dowanol DM (HD)	164	13,000	381
Propylene Glycol (GB)	346	10,310	368
Diglyme (GB)	133	13,800	324
Tetraglyme (VX)	151	13,500	527
<i>Agents</i>			
HD	169	7,340	423
GB	144	8,710	316
VX	141	13,150	568

and will vaporize slower (lower heat of vaporization) than will GB. An example of a better simulant for GB would be diethylene glycol dimethyl ether (Diglyme). Its boiling point is only 8°F higher, and its heat of vaporization is only 11 Btu/lb<sup>a</sup> lower. By using the above logic, the following simulants were also selected; for HD, diethylene glycol methyl ether (Dowanol DM) and for VX, tetraethylene glycol dimethyl ether (Tetraglyme). The above agent simulants are all simple compounds containing only C, H, and O and are readily available from commercial sources.

The third physical property which is important to consider is the heat of combustion. Note that the heat of combustion of HD and GB and their recommended simulants differ substantially. To ensure that the heat released into the furnace by the simulant is representative of the agent, the amount of simulant loaded into the furnace needs to be adjusted. For the HD and GB simulants the weight introduced into the furnace is much less than that of the agent. This is due to the lower heat of combustion of HD and GB in comparison to their simulants. The VX simulant weight is close to that of the agent VX, since the heats of combustion of the simulant and the agent are close.

### 3. MPF mathematical model

A mathematical model of the agent vaporization process from a munition was developed in order to compare the vaporization profiles for the agents and their respective simulants and to predict the performance of the MPF under various operating scenarios. Figures 2 and 3 illustrate the basic features of the munition vaporization model for projectiles and for bulk items, respectively.

The munitions are loaded into the furnace on a tray which can contain as few as 27 8-inch projectiles or as many as 96 105-mm projectiles. Bulk items typically only have 1 or 2 items on a tray. Clearly each munition will have its own unique temperature history and vaporization rate depending on its location within the tray. To account for position on the tray the munitions were grouped into six categories as shown in Fig. 2 for the 8 inch projectiles. This was done since many of the munitions on the tray see the same heat transfer environment and would be expected to heat at similar rates. This greatly simplifies the problem and speeds up the calculation considerably.

The basis of the MPF simulation is a model for the munition. Rather than solve Fourier's heat conduction equation for the temperature distribution in the munition body, a simpler approach was taken. The lumped temperature approach described below is somewhat justified because of the thinness and the high thermal conductivity of the munition metal parts. It should be pointed out that the simpler munition model was compared to a more rigorous finite-difference solution of the heat conduction equation and the difference in the

---

<sup>a</sup>1 Btu/lb  $\cong$  2.32 kJ/kg.





TABLE 5

## List of symbols

---

$A$	surface area
$C$	specific heat, cord length (see Fig. 3)
$d$	thickness of projectile base or bulk item shell
$F$	radiation view factor
$h$	heat transfer coefficient, agent depth
$H_{\text{VAP}}$	heat of vaporization
$K$	agent cross sectional area in bulk item
$L$	munition length
$m_{\text{VAP}}$	vaporization rate
$R$	radius
$T$	temperature

*Subscripts*

0	inner
1	outer
A	agent
DS	dry side
DSA	dry side to agent
DSG	dry side to gas
DSI	dry side interior
DT	dry top
DTA	dry top to agent
DTG	dry top to gas
F	furnace
FDS	furnace to dry side
FDT	furnace to dry top
FWB	furnace to wet bottom
FWBS	furnace to wet bottom side
FWS	furnace to wet side
G	gas space
GA	gas to agent
S	munition body
WB	wet bottom
WBA	wet bottom to agent
WBI	wet bottom interior
WS	wet side
WSA	wet side to agent
WSI	wet side interior

*Greek symbols*

$\rho$	density
$\sigma$	Stefan-Boltzmann constant of heat radiation
$\theta$	angle defined in Fig. 3

---

Table 5):

*dry metal sides* ( $T_{DS}$ )

$$\begin{aligned} \rho_S A_{DT} C_S \frac{d}{dt} [(L-h) T_{DS}] &= A_{DS} h_{FDS} (T_F - T_{DS}) \\ &+ A_{DS} \sigma F_{FDS} (T_F^4 - T_{DS}^4) + A_{DT} \sigma F_{FDT} (T_F^4 - T_{DS}^4) \\ &- A_{DSI} h_{DSG} (T_{DS} - T_G) - A_A \sigma F_{DSA} (T_{DS}^4 - T_A^4), \end{aligned} \quad (1)$$

*wet metal sides* ( $T_{WS}$ )

$$\begin{aligned} \rho_S A_{DT} C_S \frac{d}{dt} (h T_{WS}) &= A_{WS} h_{FWS} (T_F - T_{WS}) \\ &+ A_{WS} \sigma F_{FWS} (T_F^4 - T_{WS}^4) - A_{WSI} h_{WSA} (T_{WS} - T_A), \end{aligned} \quad (2)$$

*wet metal bottom* ( $T_{WB}$ )

$$\begin{aligned} A_{WB} d \rho_S C_S \frac{d}{dt} T_{WB} &= A_{WB} h_{FWB} (T_F - T_{WB}) + A_{WB} \sigma \\ &\times F_{FWB} (T_F^4 - T_{WB}^4) + 2\pi R_1 d \sigma F_{FWBS} (T_F^4 - T_{WB}^4) \\ &- A_{WBI} h_{WBA} (T_{WB} - T_A), \end{aligned} \quad (3)$$

*agent* ( $T_A$ )

$$\begin{aligned} \rho_A C_A A_{WBI} \frac{d}{dt} (h T_A) &= A_{WSI} h_{WSA} (T_{WS} - T_A) + A_{WBI} \\ &\times h_{WBA} (T_{WB} - T_A) + A_A \sigma F_{DSA} (T_{DS}^4 - T_A^4) + A_A h_{GA} \\ &\times (T_G - T_A) - A_A m_{VAP} H_{VAP}, \end{aligned} \quad (4)$$

*gas space* ( $T_G$ )

$$T_G = \frac{(A_{DSI} h_{DSG} T_{DS} + A_A m_{VAP} C_{AG} T_A + A_A h_{GA} T_A)}{(A_{DSI} h_{DSG} + A_A m_{VAP} C_{AG} + A_A h_{GA})} \quad (5)$$

The agent mass balance is also given by

$$\rho_A \frac{dh}{dt} = -m_{VAP} \quad . \quad (6)$$

With the length of the munition represented by  $L$ , its inner radius by  $R_0$ , its outer radius by  $R_1$ , and the thickness of the base by  $d$ , the following equations then represent the various heat transfer areas

*area of wet bottom*

$$A_A = A_{WBI} = \pi R_0^2, \quad A_{WBE} = \pi R_1^2,$$

area of wet sides

$$A_{WSI} = 2\pi R_0 h(t), \quad A_{WSE} = 2\pi R_1 h(t),$$

area of dry sides

$$A_{DSI} = 2\pi R_0 (L - h(t)), \quad A_{DSE} = 2\pi R_1 (L - h(t)),$$

area of dry top

$$A_{DT} = \pi(R_1^2 - R_0^2).$$

Figure 3 illustrates the basis of the model for bulk items such as the ton container. The bulk item is placed on the tray in a horizontal orientation. Because of this placement, the agent surface area will depend on the angle ( $\theta$ ) formed between the centerline of the bulk item and the ends of the exposed agent interface. The regions of the bulk item are the dry top, the dry sides, the wet bottom, and the wet sides. The gas space above the agent and the agent

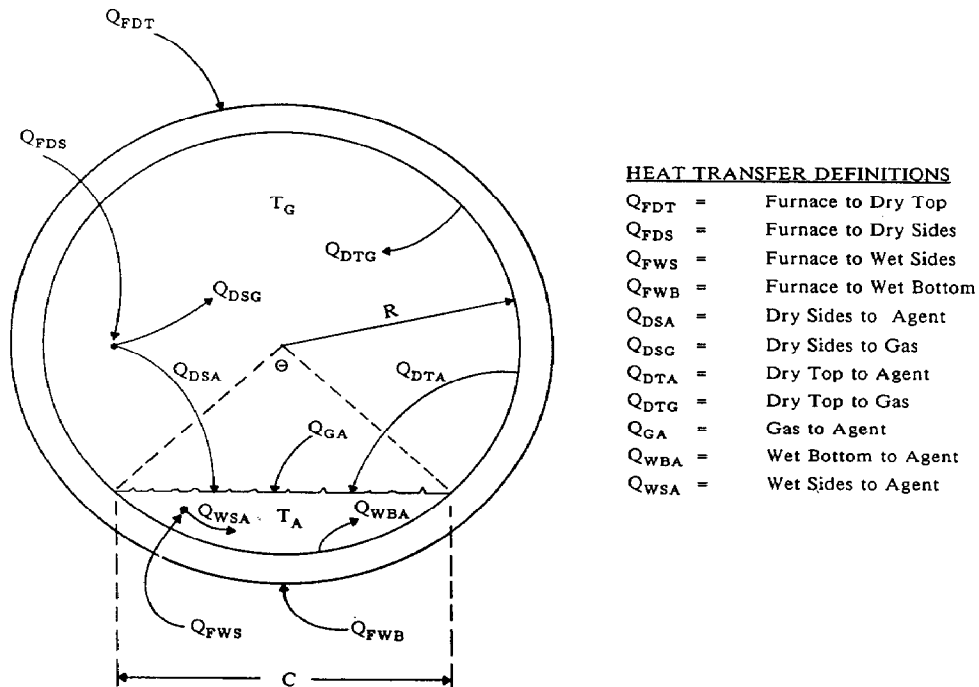


Fig. 3. Bulk item vaporization model.

itself are also considered as separate regions. The following equations can be written to describe the temperature in each of these regions:

*dry metal top* ( $T_{DT}$ )

$$\begin{aligned} \rho_S dC_S \frac{d}{dt} [A_{DT} T_{DT}] &= A_{DT} h_{FDT} (T_F - T_{DT}) + A_{DT} \sigma F_{FDT} \\ &\times (T_F^4 - T_{DT}^4) - A_{DT} h_{DTG} (T_{DT} - T_G) - A_A \sigma F_{DTA} \\ &\times (T_{DT}^4 - T_A^4), \end{aligned} \quad (7)$$

*dry metal sides* ( $T_{DS}$ )

$$\begin{aligned} \rho_S dC_S \frac{d}{dt} [A_{DS} T_{DS}] &= A_{DS} h_{FDS} (T_F - T_{DS}) + A_{DS} \sigma F_{FDS} \\ &\times (T_F^4 - T_{DS}^4) - A_{DS} h_{DSG} (T_{DS} - T_G) - A_A \sigma F_{DSA} \\ &\times (T_{DS}^4 - T_A^4), \end{aligned} \quad (8)$$

*wet metal bottom* ( $T_{WB}$ )

$$\begin{aligned} \rho_S dC_S \frac{d}{dt} [A_{WB} T_{WB}] &= A_{WB} h_{FWB} (T_F - T_{WB}) + A_{WB} \sigma F_{FWB} \\ &\times (T_F^4 - T_{WB}^4) - A_{WB} h_{WBA} (T_{WB} - T_A), \end{aligned} \quad (9)$$

*wet metal sides* ( $T_{WS}$ )

$$\begin{aligned} \rho_S dC_S \frac{d}{dt} [A_{WS} T_{WS}] &= A_{WS} h_{FWS} (T_F - T_{WS}) + A_{WS} \sigma F_{FWS} \\ &\times (T_F^4 - T_{WS}^4) - A_{WS} h_{WSA} (T_{WS} - T_A), \end{aligned} \quad (10)$$

*agent* ( $T_A$ )

$$\begin{aligned} L\rho_A C_A \frac{d}{dt} [KT_A] &= A_{WS} h_{WSA} (T_{WS} - T_A) + A_{WB} h_{WBA} (T_{WB} - T_A) \\ &+ A_A \sigma F_{DSA} (T_{DS}^4 - T_A^4) + A_A \sigma F_{DTA} (T_{DT}^4 - T_A^4) \\ &+ A_A h_{GA} (T_G - T_A) - A_A m_{VAP} H_{VAP}, \end{aligned} \quad (11)$$

*gas space* ( $T_G$ )

$$T_G = \frac{(A_{DT} h_{DTG} T_{DT} + A_{DS} h_{DSG} T_{DS} + A_A m_{VAP} C_{AG} T_A + A_A h_{GA} T_A)}{(A_{DT} h_{DTG} + A_{DS} h_{DSG} + A_A m_{VAP} C_{AG} + A_A h_{GA})}. \quad (12)$$

The agent mass balance is written as

$$\rho_A \frac{dK}{dt} = -m_{VAP} C. \quad (13)$$

With the length of the bulk item given by  $L$ , its radius by  $R$ , and the thickness of its shell by  $d$ , the following equations provide the various heat transfer areas:

*cross sectional area of the agent*

$$K = 0.5 R^2 (\Theta - \sin \Theta), \text{ for less than half full,}$$

*area of the dry top*

$$A_{DT} = RL(2\pi - \Theta),$$

*area of the dry sides*

$$A_{DS} = 2(\pi R^2 - K),$$

*area of wet bottom*

$$A_{WR} = R L \Theta,$$

*area of wet sides*

$$A_{WS} = 2 K,$$

*exposed area of agent*

$$A_A = 2 R L \sin(0.5 \Theta),$$

*cord length*

$$C = 2 R \sin(0.5 \Theta).$$

The heat transfer coefficients represented by the subscripted  $h$  terms, and the radiation view factors represented by the subscripted  $F$  terms, were obtained from literature correlations. The terms  $h_{WSA}$  and  $h_{WBA}$  will change from convective heat transfer coefficients to boiling heat transfer coefficients once the agent reaches its boiling point. When the agent temperature is below its boiling point, the last term in the agent energy equation represents energy lost due to agent mass transfer. When the agent reaches its boiling temperature the left hand side of this equation is zero and the agent energy equation can be solved for the agent vaporization rate.

The above equations were numerically integrated to obtain the vaporization rate as a function of time. The furnace temperature,  $T_F$ , was assumed to be known as a function of time and was not obtained by a separate energy balance on the furnace. All required physical properties for the agents and their simulants were obtained from published data or estimated by using the methods outlined in Reid et al. [3].

#### 4. Results and discussion

Figures 4–9 present actual test results from the CAMDS MPF when processing ton containers containing a 5% by weight heel of agent simulants. The

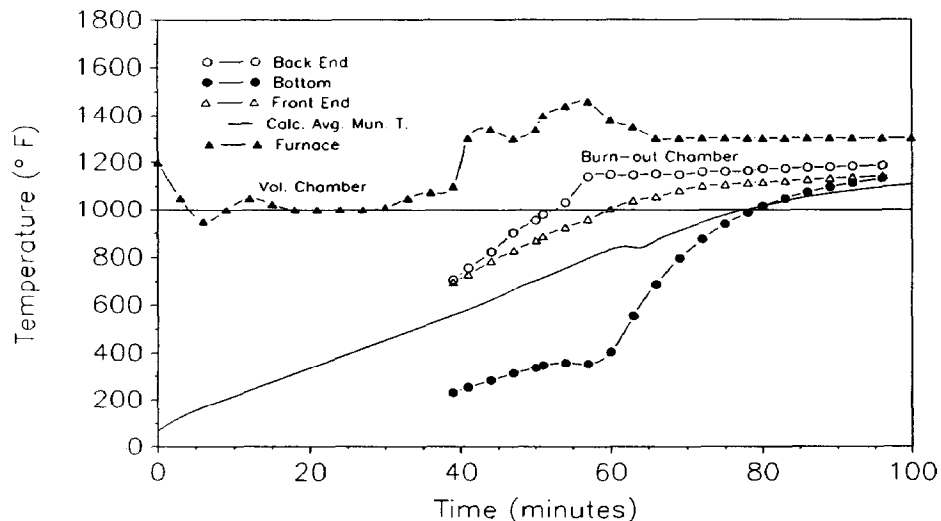


Fig. 4. Ton container test; temperature data, 5% Heel of Dowanol DM.

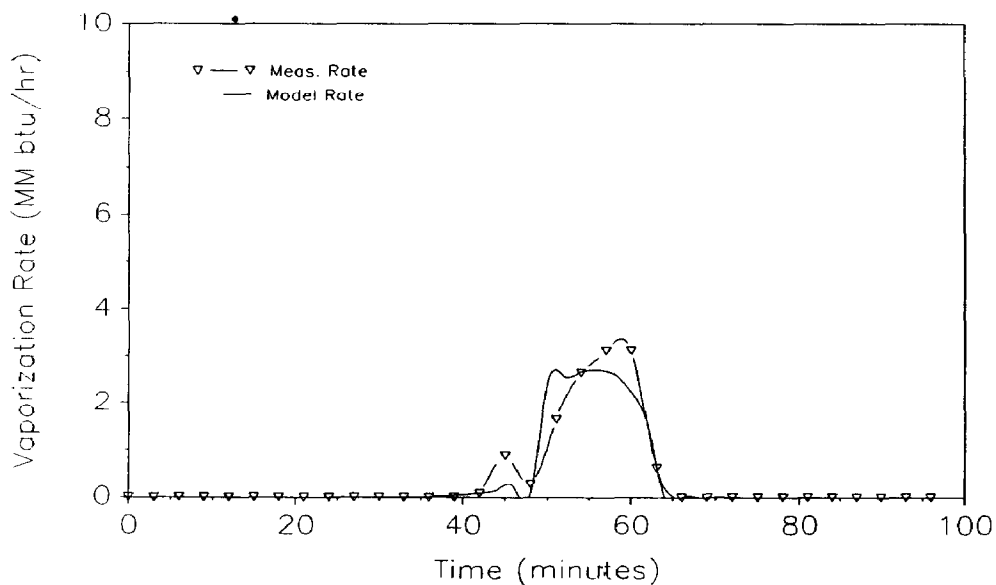


Fig. 5. Ton container test; vaporization data, 5% Heel of Dowanol DM.

simulant vaporization rate was calculated from data which included the total fuel oil flow to the furnace, and the analysis of the flue gas for carbon dioxide, carbon monoxide, hydrocarbons, and oxygen. As the vaporization rate increases, the furnace temperature controller reduces the fuel flow to maintain constant furnace temperature. When the fuel oil is turned down, the oxygen

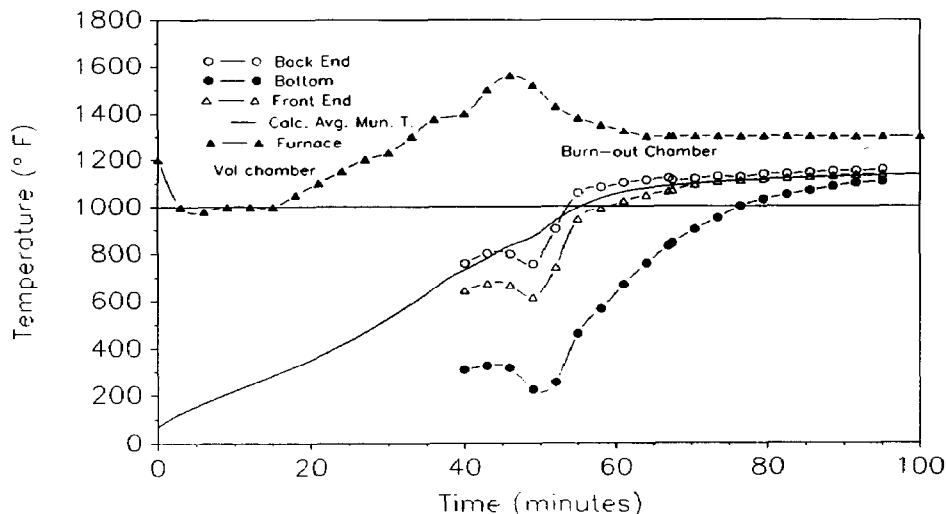


Fig. 6. Ton container test; temperature data, 5% Heel of Diglyme.

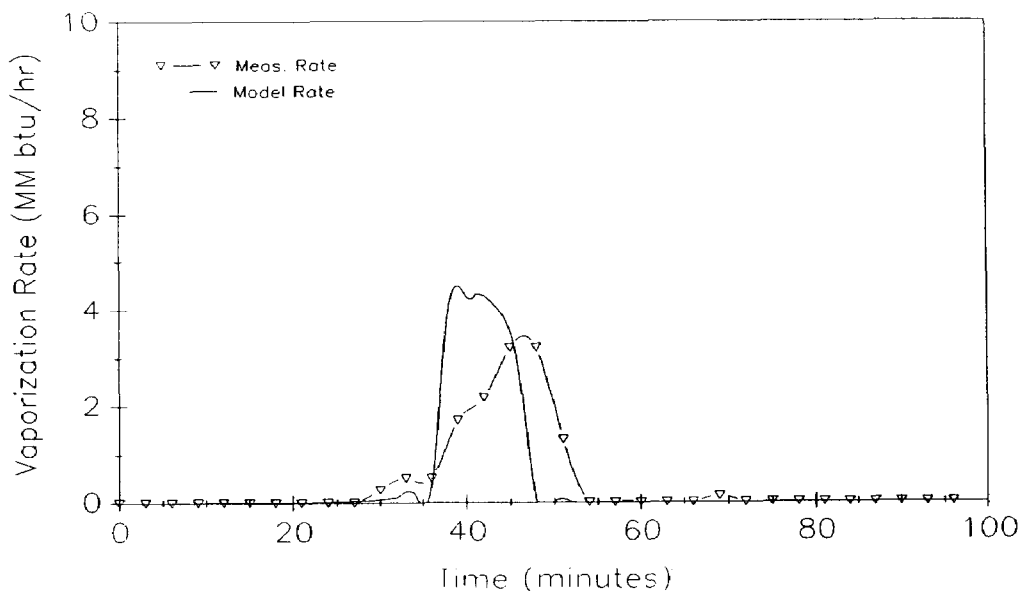


Fig. 7. Ton container test; vaporization data, 5% Heel of Diglyme.

concentration drops, and the carbon dioxide rises due to continued combustion of the simulant. The rate of change of the fuel oil flow rate, and finally of the oxygen concentration can be correlated through the simulant combustion reaction stoichiometry to the rate of simulant vaporization. Also shown in the



figures are the predicted simulant vaporization rate and average munition temperature by using the model described above. Good agreement between the model and the actual data was obtained for the munition heating rate in all cases. Excellent agreement between the model and the actual data was obtained for the vaporization rate of Dowanol DM (HD simulant), and Diglyme (GB simulant). The starting time for vaporization, the peak vaporization rate, and the duration of vaporization were in excellent agreement. For Tetraglyme (VX simulant), the model did not agree with the furnace data (see Figs. 8 and 9). The furnace data shows the vaporization rate to slowly increase to the peak value starting much earlier than the predicted onset. This slow increase is atypical of simulant vaporization (compare the vaporization rate profiles to that of Dowanol DM and Diglyme). The profile for Tetraglyme suggests a slowly increasing decomposition rate to more volatile products as the temperature of the ton container bottom increases. The temperature of the ton container bottom also suggests non-uniform boiling or decomposition. Rather than moving rapidly to the boiling point of Tetraglyme and holding there, as it does for the other simulants, the temperature at the container bottom slowly climbs toward the boiling point of Tetraglyme (527°F), then rapidly increases when the simulant has evaporated. The behavior of Tetraglyme in the furnace may actually fit that of VX. Data presented in Ref. [1] indicates that VX could be expected to decompose within the MPF.

Figures 10–12 compare the predicted vaporization rates for three projectile munition types containing the agent and its simulant. The munitions were assumed to contain a 5% by weight of agent heel. For the projectile runs the

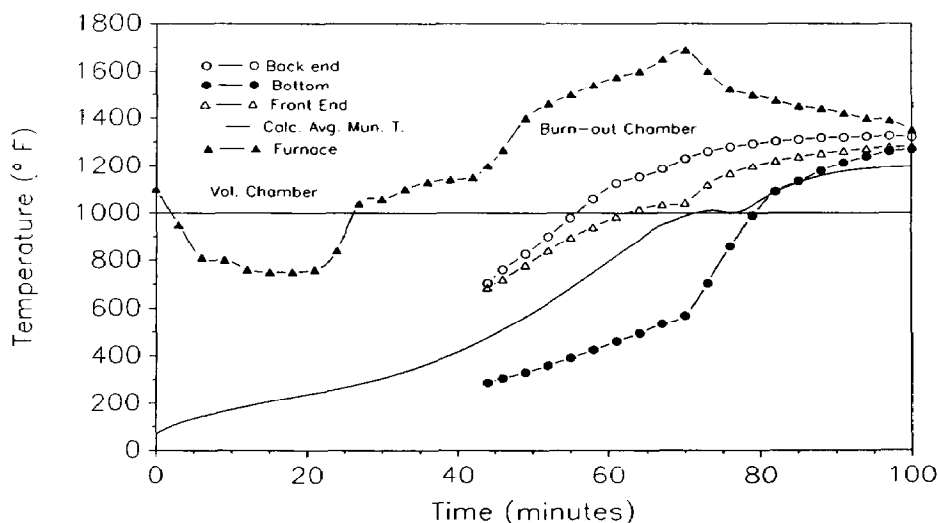


Fig. 8. Ton container test; temperature data, 5% Heel of Tetraglyme.

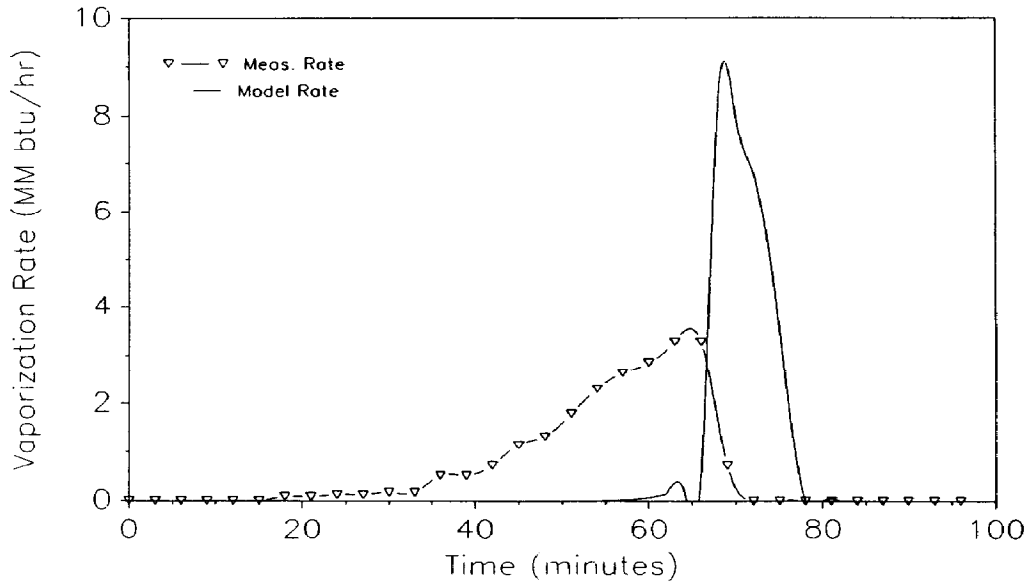


Fig. 9. Ton container test; vaporization data, 5% Heel of Tetraglyme.

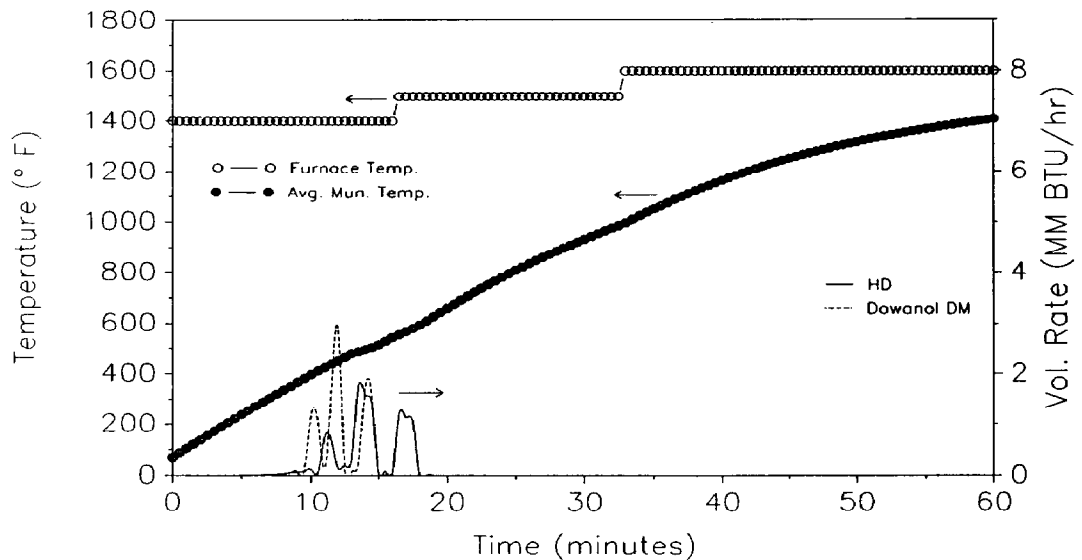


Fig. 10. Metal parts simulation; 105-mm projectiles, 5% Heel of HD and Dowanol DM.

furnace temperature was stepped from 1400 to 1600°F as the munition moves through the furnace's three zones. As discussed earlier, the amount of simulant loaded was adjusted to provide the same total heat release as its respective

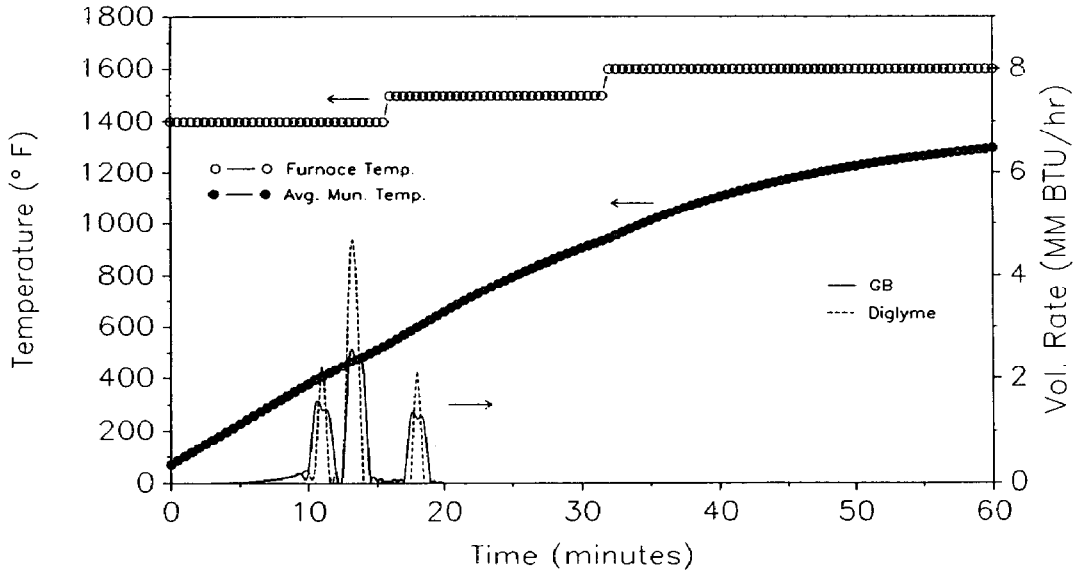


Fig. 11. Metal parts simulation; 155-mm projectiles, 5% Heel of GB and Diglyme.

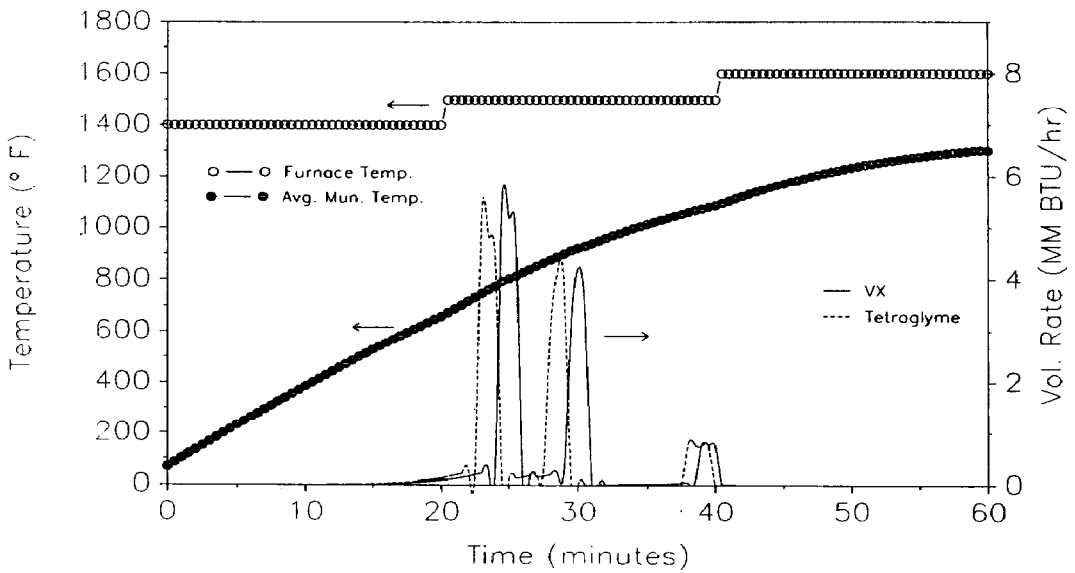


Fig. 12. Metal parts simulation; 8-inch projectiles, 5% Heel of VX and Tetraglyme.

agent. It is also interesting to note for the projectiles the peak and valley nature of the vaporization process. This results from the different heating rates of the munition categories as discussed earlier.

The figures show excellent correlation of the predicted onset of the vapori-

zation process for each of the agents and their simulants. This is expected, since, as shown in Table 4, good agreement was obtained between the agent and simulant boiling points. The peak vaporization rates and duration of vaporization for the agents and their simulants are also in excellent agreement and this reflects the closeness between the heat of vaporization for these materials. The duration of vaporization for the simulants is somewhat shorter, which results from the fact that less simulant was added to the munition in order to match the total heat release of the agent. For mustard and GB the peak energy release rates for their simulants are somewhat higher than for their corresponding agents. The higher peak energy release of the simulants is somewhat beneficial in that if the furnace can handle these rates for the simulants, it should easily process the lower peak rates of the agents themselves.

## 5. Conclusions

The results of this study show how simulants for a hazardous material, in this case chemical warfare agents, can be rationally selected on the basis of physical properties and mathematical modelling. Predictions of the vaporization rates by using the MPF model show that the agents and their simulants have nearly identical vaporization rate profiles and can be confidently used to test the furnace operating characteristics. Testing of simulants in ton containers in the CAMDS MPF was successful and verified the MPF model for ton containers. The MPF model can now be used to confidently predict the operating characteristics of the MPF when processing ton containers with the actual chemical agents. As shown in this study simulants can be used to safely test and fine-tune the operating conditions of hazardous waste incineration systems without the risk associated with using the actual hazardous material.

## References

- 1 US Army FM 3-9, Headquarters, Military Chemistry and Chemical Compounds, Department of the Army, October 1975.
- 2 R. Rife, T. Thomas, R. Fournier, D. Norberg, M. Bonomo, and F. Rinker, Chemical demilitarization: Disposing of the most hazardous wastes, *Environ. Progr.*, 8(3) (1989) 167-175.
- 3 R.C. Reid, V.M. Prausnitz and B.E. Poling (Eds.). *The Properties of Gases and Liquids*, 4th ed. McGraw-Hill, New York, NY, 1987.