Advanced Modeling of Incineration of Building Decontamination Residue

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ABSTRACT

In this paper we present recent development of the component models for a pilot scale rotary kiln simulator for the incineration of building materials. A transient zonal model approach for use with a computational fluid dynamics (CFD) model is presented. Comparisons are made between the model and experimental data. The models predict complete destruction of the biological agent that remains in the building material matrix when the incinerators and afterburners are operated as per standard operating.

NOMENCLATURE

A Arrhenius preexponential constant, 1/s

C_p Specific heat, J/kg/K

C Z value form preexponential constant, 1/s

E/R Arrhenius activation energy to gas constant ratio, K

f_i Mass fraction of ith stream

h Enthalpy, J/kg

k Thermal Conductivity, W/m/K

$\dot{m}$ Mass flow rate, kg/s

Q_c Convective heat transfer, W

Q_r Radiative heat transfer, W

t Time, s

V Volume, m^3

y Viable spores

Y_i Devolatilization yield

Z Z value, K

T Temperature, K

ρ Density, kg/m^3

NOTATION

CFD	Computational Fluid Dynamics
CWA	Chemical Warfare Agents
DFS	Deactivation Furnace System
GB	Sarin
HD	Mustard Agent
REI	Reaction Engineering International
VX	VX nerve gas

INTRODUCTION

The EPA National Homeland Security Research Center (NHSRC) has initiated research to develop better methods, technologies, and guidance relating to building decontamination in the event of a terror attack. Incineration is one of the primary technologies being studied for the disposal of contaminated building materials. As part of that effort, Reaction Engineering International (REI), under contract to EPA, is developing computer simulation tools for analyzing incinerators processing building material contaminated by biological weapon (BW) agents or chemical weapon (CW) agents. These agents are collectively termed chemical/biological (CB) agents. The model results are being compared against pilot-scale data collected by EPA to characterize the behavior of BW agents, as would be found in a structure, bound in various matrices and materials, typical of an office building/environment.

The models being developed will take advantage of a Department of Defense (DoD) Small Business Innovative Research (SBIR) program recently completed[1-4] by REI to develop a suite of models for conducting detailed simulations of chemical demilitarization incinerator operation. As part of that SBIR project, computational chemistry methods were used to develop detailed chemical kinetic mechanisms to describe the decomposition of CW agents of mustard (HD), and nerve agents GB and VX.

The purpose of the modeling effort is to provide facilities and permitting agencies to perform "what if" type scenarios to assess the effect of operating conditions on destruction of CB agents. In addition, by being able to simulate incinerator failure modes, risk assessors can analyze situations such as the impact of power loss and system shutdown while CB agents are in the incinerator.

Ultimately, the models are to be used to extrapolate heat transfer, fluid dynamics, and chemical kinetic behavior to characterize the full-scale effect. Models for full-scale incinerators under development include an oxygen starved medical waste incinerator and a commercial scale rotary kiln incinerator. As part of this effort a model has been developed for the pilot-scale rotary kiln simulator at the EPA NHSRC. The development of this laboratory kiln model is the focus of this paper. The modeling approach for the incinerators is discussed. The kinetic models for BW agents are developed and comparisons are made with the laboratory data. Finally, comparison with laboratory scale kiln data is made.

ROTARY KILN SIMULATOR DESCRIPTION

Testing was performed at the EPA's Rotary Kiln Incinerator Simulator (RKIS) facility located in Research Triangle Park, NC. The RKIS (shown in Figure 1) consists of a 73 kW (250,000 Btu/hr) natural gas-fired rotary kiln section and a 73 kW (250,000 Btu/hr) natural gas-fired secondary combustion chamber (SCC). Following the SCC is a long duct that leads into a dedicated flue gas cleaning system (FGCS) consisting of another afterburner, baghouse, and wet scrubber. The RKIS is equipped with continuous emission monitors (CEMs) for oxygen (O_2), carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NO_x), and total hydrocarbons (THCs). A series of Type-K thermocouples monitor the temperature throughout the system. For the data reported here, the rotary kiln combustion air was flowing at a rate of 82.4 sm^3/hr (2909 scfh) and the burner natural gas fuel was flowing at a rate of 5.66 sm^3/hr (200 scfh). The static pressure in the rotary kiln section was maintained at -0.05 in. w.c. The typical gas residence times are 2 seconds in the kiln, 3 seconds in the transition between the kiln and secondary combustion chamber, and 7 to 8 seconds in the secondary combustion chamber. The typical residence time for the solid matrix material is 10 minutes. This facility has been used for testing a variety of wastes[5].
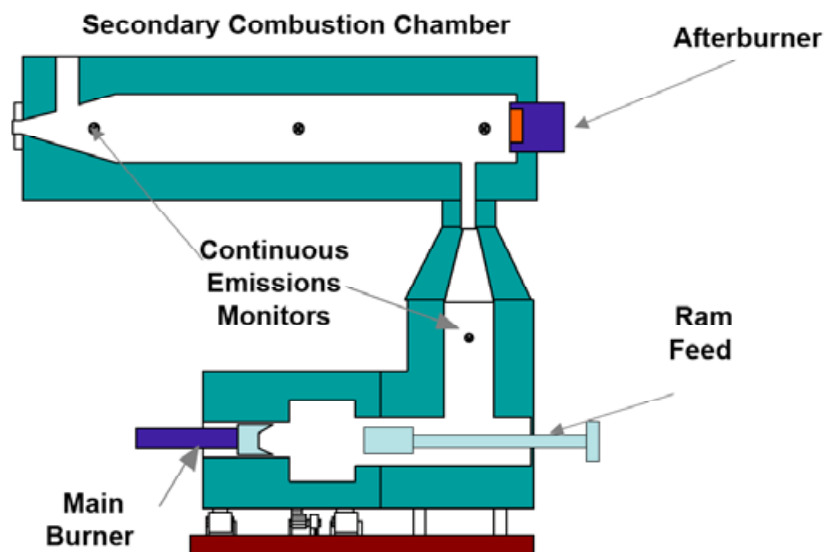

Figure 1. Rotary Kiln Incinerator Simulator.

MODELING APPROACH

In the kiln, the periodic loading of building materials results in an inherently time dependent operation that must be adequately captured in the model. Modeling the operation with a true transient computational fluid dynamics (CFD) simulation would require excessive computing resources. To better represent the time dependent nature of the kiln in an efficient manner, we use a combination of a transient "zonal" model and a steady state CFD model. The transient zonal model captures the transient effect of building matrix combustion, on the furnace temperature and overall gas composition. A steady state 3D CFD model is used to compute the local mixing and destruction efficiency for a prescribed instant in time. The BW agent destruction can be tracked within the matrix or traced along streamlines for spores released into

the gas. The release rate of spores is not calculated in the model but rather the log reduction along gas phase streamlines of any spores that may be released. Chemical agent vaporization is modeled and destruction is assumed to occur in the gas after release. A key aspect is that the matrix combustion rate and wall thermal behavior determined with the transient zonal models are used to define the boundary conditions, required by the CFD model. This paper focuses on the zonal model and BW destruction in the matrix.

Transient Kiln Zonal Model

The transient zonal model consists of a gas phase zonal combustion submodel and a matrix combustion model. The gas temperature and composition of each zone is assumed uniform. Ordinary differential equations (ODE's) are integrated over time representing the material and energy balances of the gas phase of each zone and the agent within each individual projectile. The following ODE governs the material balance in each zone:

$$\frac{df_i}{dt} = \frac{1}{\rho V}\left(-f_i V \frac{d\rho}{dt} - \dot{m}_{out} f_i + \sum_{in} \dot{m}_{in} f_{i,in}\right) \qquad (1)$$

where f_i is the mass fraction of the ith stream, V is the zone volume, and ρ is the gas density. The mass fraction of the various streams represents the elemental composition of the gas for use in equilibrium calculations. The streams tracked are the fuel such as natural gas, dry ash-free matrix fuel, air, and water. The mass flow rates, $\dot{m}_{in}$, include the off-gas of water or dry ash-free (DAF) fuel. Mass conservation for each zone is expressed as:

$$\dot{m}_{out} = \sum_{in} \dot{m}_{in} - V \frac{d\rho}{dt}. \qquad (2)$$

The following gas enthalpy equation for each zone is also integrated:

$$\frac{dh}{dt} = \frac{1}{\rho V}\left(-hV \frac{d\rho}{dt} - \dot{m}_{out} h + \sum_{in} \dot{m}_{in} h_{in} + Q_c + Q_r\right) \qquad (3)$$

where Q_c and Q_r represents the convective and radiative heat transfer in the zone, respectively. Continuity, Equation (2), may be substituted into Equations (1) and (3) to simplify those expressions.

For each matrix piece, partial differential equations (PDE's) for the distribution of the matrix temperature, mass, and material (water, DAF fuel, char and ash) are also integrated. The temperature distribution within the matrix is governed by the thermal diffusion equation.

$$\frac{\partial T}{\partial t} = \frac{1}{\rho C_p} \nabla \cdot k \nabla T \qquad (4)$$

The matrix, which is assumed to be a rectangular box in geometry, is discretized in three directions. The processes of drying, devolatilization, and char oxidation are also modeled. The drying process is modeled as a two-step procedure[6]: 1) when the moisture content of the matrix is higher than certain critical value, the temperature increase of the matrix is minimal. Thus the water evaporation rate is calculated based on the heat flux into the matrix, and the moisture mass fraction is assumed to be uniform. 2) When the moisture mass fraction is lower than the critical value, the temperature of the matrix start to increase. We assume that the surface evaporation

rate is much smaller than the boiling evaporation rate and is neglected in the drying process. The devolatilization process is modeled as a two-step reaction:

$$C_{daf} \xrightarrow{\ k_i\ } Y_i \, \text{Vol} + (1 - Y_i) \, \text{Char}, \qquad i = 1,2$$
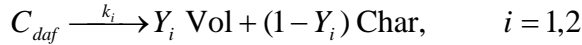
For the results presented in this paper, k_2 is assumed to be 0 therefore producing a fixed volatile yield. A global model based on the first order oxygen and total matrix surface area is employed for modeling of char oxidization rate.

The model is advanced through time using a 4th order Runge-Kutta time stepping scheme with adaptive time step size control[7] to maintain prescribed accuracy tolerances. At each time step the zones are updated with upstream zones first. The zone containing the outlet duct to the afterburner is updated last. At each time step a chemical equilibrium calculation is performed to obtain the zone furnace gas temperature and composition from the stream mass fractions and enthalpy.

Output from the transient model includes as a function of time the temperature distribution within each matrix piece, matrix volatile release and char production rate, char oxidation rate, furnace gas temperature and gas composition. The vaporization rate and the burner, drying, matrix combustion, and airflow rates are used as inputs (boundary conditions) to the 3D CFD model of the kiln.

BW Agent Thermal Destruction Kinetics Development

Destruction of BW agent with temperature involves complex processes of microbiology. In order to have a predictive tool to provide spore destruction trends within an incinerator a kinetic model must be developed. In this paper the destruction is assumed to be first order

$$\frac{dy}{dt} = -ky \tag{5}$$

where y represents the number of viable spores and k is the kinetic rate constant which is function of temperature. The log reduction of viable spores for given time of exposure at temperature T for a first order rate is then given as

$$\log reduction = \log_{10}\left(\frac{y_0}{y}\right) = \frac{k(T)t}{\ln 10} \tag{6}$$

where y_0 is the initial amount of viable spores. The form of the rate constant as a function of temperature is next needed. The concept of the Z value from microbiology[8] is used as guidance in providing this form. If D is the time required at a given temperature to achieve a log reduction in organisms, then Z is defined as the number of degrees change in temperature needed to change the D value by a factor of 10. For example, if Z is 10 degrees F, and if D is 5 minutes at 130F, then D will be 50 minutes at 120F. It follows that $Z = T_2 - T_1$ if

$$\log reduction = \log_{10}\left(\frac{y_0}{y}\right) = \frac{k(T_2)D}{\ln 10} = \frac{k(T_1)10D}{\ln 10} . \tag{7}$$

If the Z value is assumed constant the following form will satisfy Eq. 7.

$$k = Ce^{\frac{\ln 10}{Z}T} \ .$$
(8)

Here C is the preexponential constant. Alternatively, an Arrhenius form may be borrowed from chemical kinetics.

$$k = Ae^{-\frac{E}{RT}}$$
(9)

where E is the activation energy, R is the gas constant and A is the preexponential constant. This form yields a Z value that is a function of the two temperatures

$$Z = \frac{\ln 10}{E/R}T_1 T_2 \ .$$
(10)

Parameters for both forms of the rate constant have been fit to data obtained by the EPA NHSRC[9]. The fit for the building material types of ceiling tile and wallboard is shown in Figures 2 and 3, respectively. Table 1 lists the fit parameters. Since the destruction is assumed first order all the fit curves are straight lines that pass through the zero time at zero log reduction. The ceiling tile data exhibit more scatter.
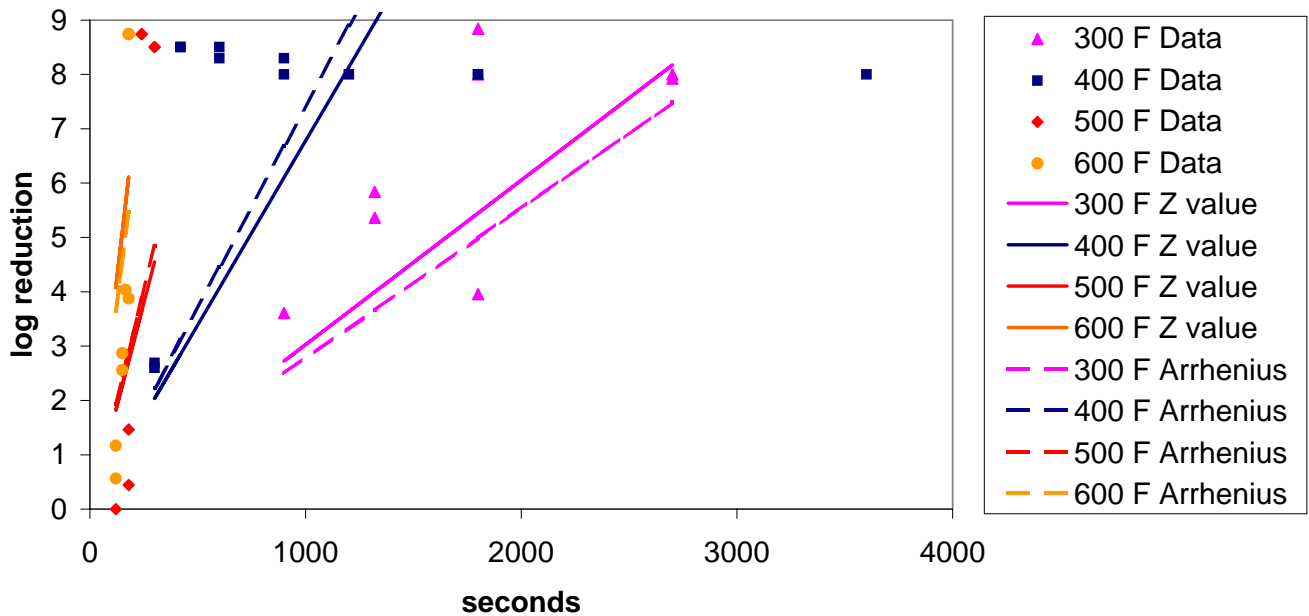

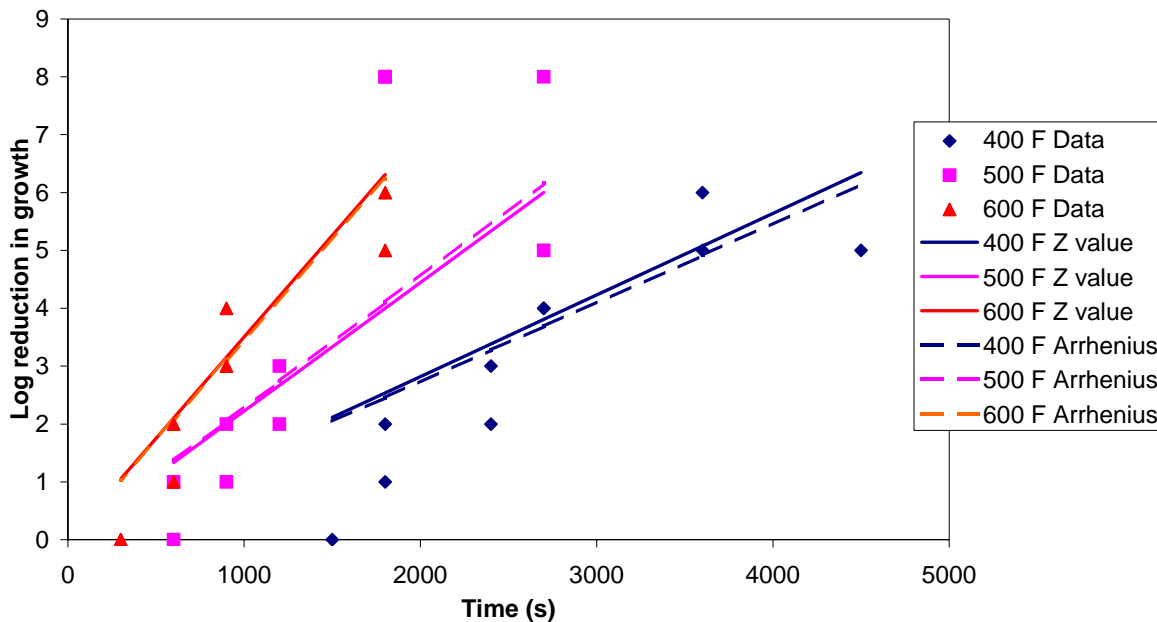Figure 2. Log reduction versus time for B. subtilis on ceiling tile at various initial temperatures.

Figure 3. Log reduction versus time for B. subtilis on wallboard at various initial temperatures.

Table 1. Kinetic BW Destruction Parameters.

	Z value		Arrhenius	
	C, 1/s	Z, K	A, 1/s	E/R, K
ceiling tile	1.534E-05	158.799	30.01	3568.3
wallboard	6.464E-05	280.803	0.435	2354.7

RESULTS

The objective of the development of the pilot scale kiln simulator model is to provide a means of calibrating the model for use in scaling up to evaluate larger systems that could be used in building residue incineration following a terror attack. Data are much more accessible in the pilot scale facility than would be in a commercial scale unit. Data were collected for processing nylon 6.6 carpet bundles in the unit by EPA and made available for testing the model. The bundles were fed about every 10.5 minutes. The bundles were approximately 50% water.

The user interface of the software has a variety of matrix property inputs as well as operating condition inputs. Matrix property inputs include matrix density, dimensions, thermal conductivity, specific heat, and surface emissivity. The analysis of the matrix is also input which includes ultimate analysis, ash content, water content, and higher heating value. Devolatilization and char oxidation parameters are also input. The parameters adjusted to produce agreement with

the temporal data set were the matrix surface emissivity and devolatilization rate parameters of the matrix.

Figures 4 and 5 show the comparison between the model calculations and the measured data of the kiln exit temperature and the SCC exit oxygen. Two successive carpet bundle dumps were modeled. The time of the first dump corresponds to zero minutes. The drop in oxygen is the result of matrix combustion. Both the model and the data show slight increases in temperature of the second dump profile compared to the first. This is the result of wall refractory being heated.
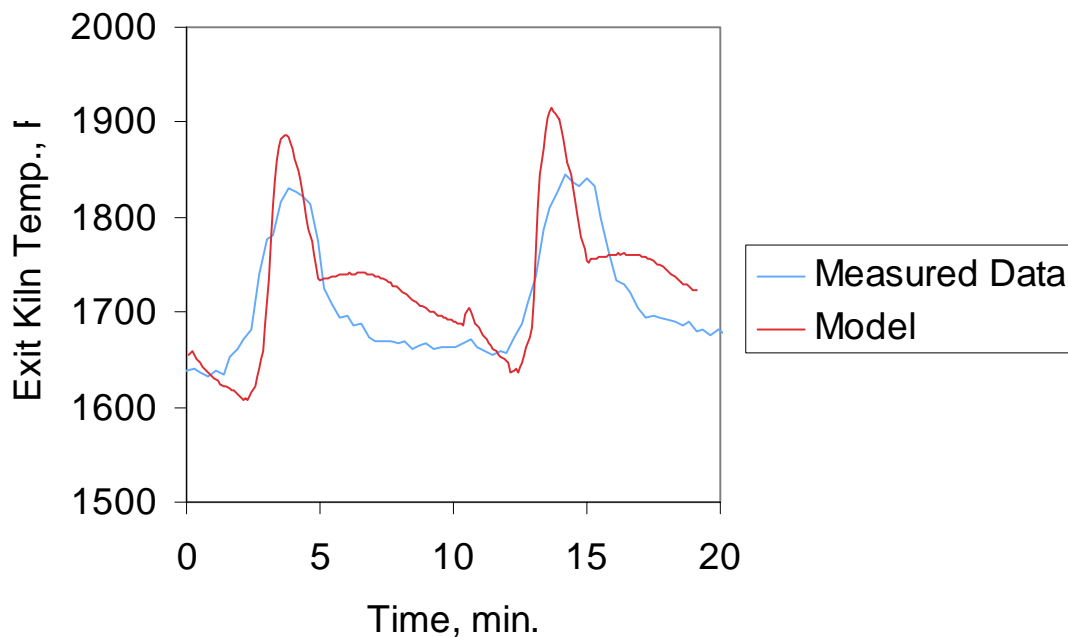

Figure 4. Comparison between measured data and model calculations of the temporal variation of the kiln exit temperature.
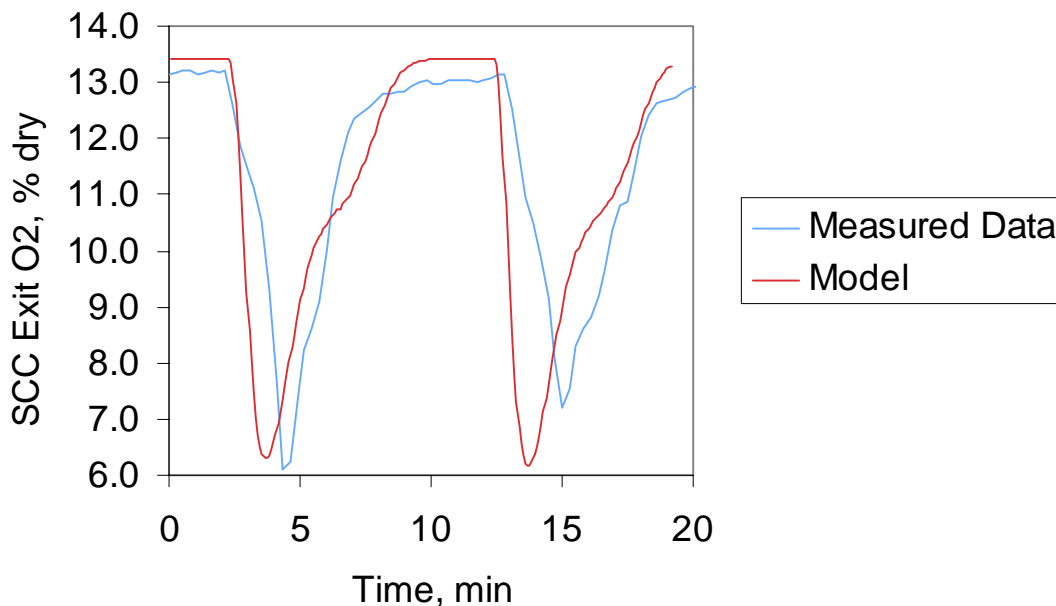

Figure 5. Comparison between measured data and model calculations of the temporal variation of the SCC exit oxygen.

The agreement between the model and the measured data is good following the adjustment of the two parameters. The emissivity of about 0.5 produced agreement with the time of completion of drying and the onset of matrix devolatilization. The devolatilization parameters thus obtained where subsequently used in a calculation and compared with weight loss data from thermal gravimetric analysis (TGA) for the nylon 6.6[10]. The calculation captured the correct overall weight loss over the temperature ramp period to within 20%. This agreement suggests that other input parameters are a fairly good representation of the actual matrix. More data such as actual temperatures within the matrix would provide a better calibration.

Since equilibrium is used in the gas combustion of the zonal model the CO is severely underpredicted. However other major species such as CO_2 are well predicted by the approach.

Figure 6 shows the spatial minimum and maximum temperatures and water mass within the first matrix as a function of time. Large gradients in temperature exist, in particular when water is present. The outer surface temperature rises very rapidly after the water has vaporized from the outer regions of the bundle.

In addition to integrating the governing ordinary and partial differential equation describing the combustion and heat transfer processes, the destruction of the BW agent within the matrix is also integrated. Figure 7 shows the log reduction of the BW agent as a function of time using both the Z value and Arrhenius form for the rate constant (Eqs. 10 and 11). The kinetic parameters used were those of *B subtillis* in ceiling tile. These parameters were used since at this writing, data for BW in carpet were not available. Although both forms provide a reasonable fit to bench scale data at low temperatures (see Figures 2 and 3), the difference between the Z value and Arrhenius predictions become more severe at very high temperatures were there is no data. It is clear that full destruction quickly ensues once a sufficient temperature has been reached. The Arrhenius
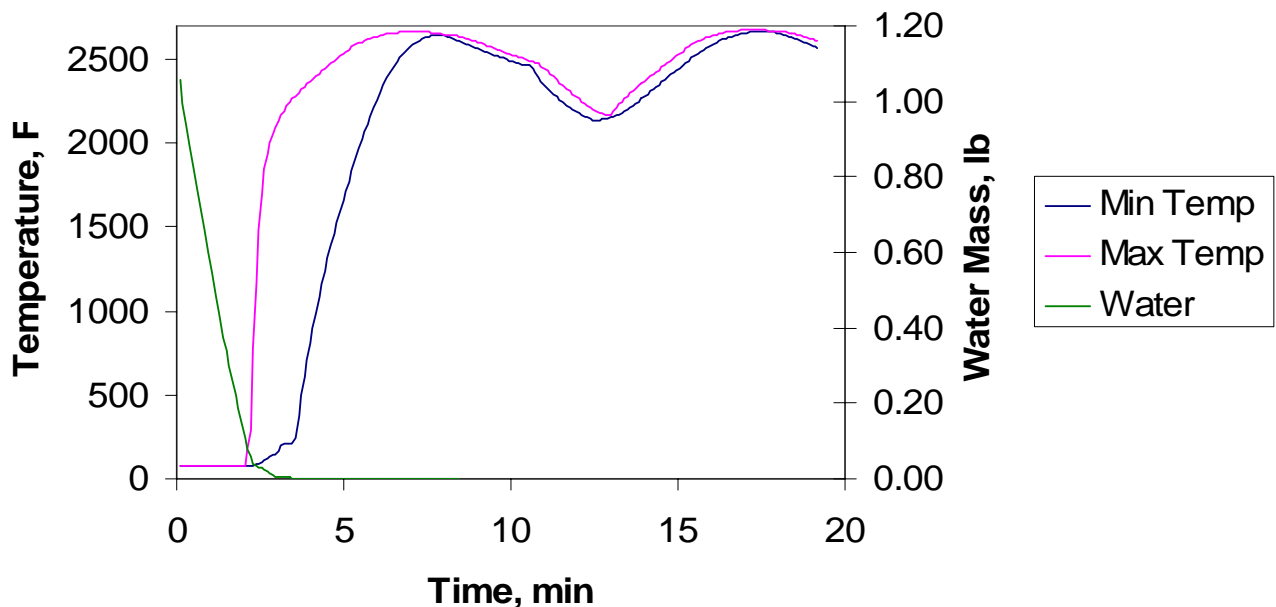

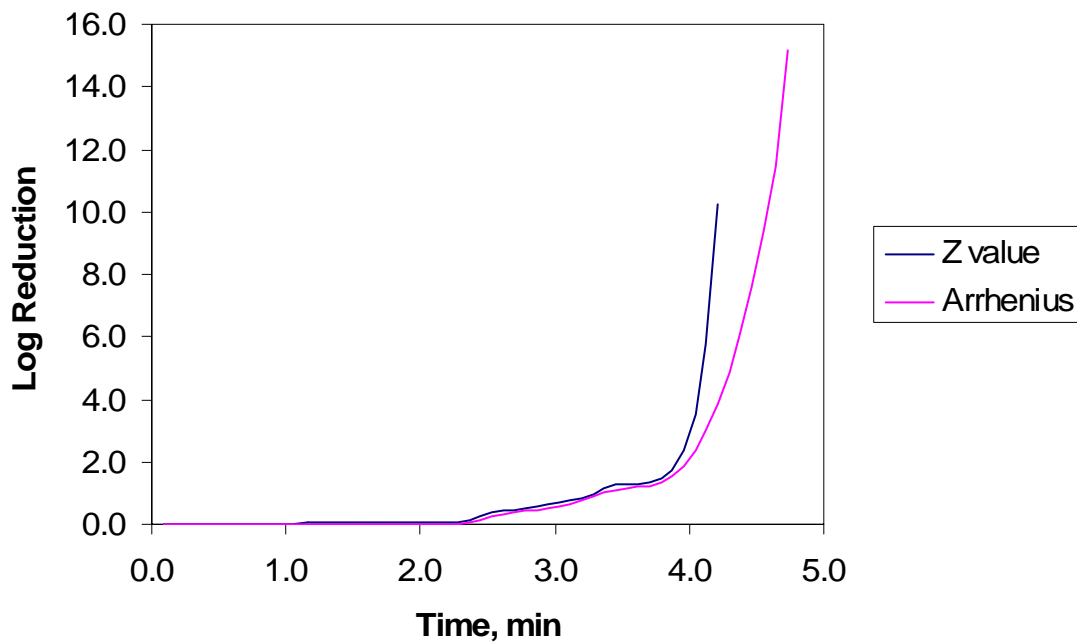Figure 6. Minimum and maximum matrix temperatures and water mass.

Figure 7. Log reduction of the biological weapons agent as calculated by the model.

expression yields the more conservative result. For the larger residence times associated with spores trapped within the matrix both forms predict full destruction. However, when tracking the destruction for spores that become entrained in the gas the resulting residence times would be much smaller, although there would be no material heat transfer barriers for spores in flight. The difference in the spatial minimum and maximum temperatures within the matrix shown in Figure 6 is indicative of such material heat transfer barriers.

CONCLUSION

This paper has demonstrated that zonal and CFD models of the laboratory scale kiln can be constructed and provide useful information on the physical processes that affect furnace performance in terms of microbiological destruction efficiency and operability. The pilot scale rotary kiln simulator model has shown useful for calibration with easily attainable data. A comparison has been made between the model and experimental kiln data obtained to provide calibration, which will permit use with full-scale incinerator models. Only data concerning operational characteristics were used in the comparison. No experimental data on biological agent destruction within the kiln were available at this writing. The models predict complete BW agent destruction for agent that remains within the matrix. The models may also be useful in simulating incineration system upset conditions and failures that could lead to an agent release, so that appropriate design and operational modifications can be made to mitigate such occurrences.

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