Agent Fate Program Activities at Kettering University

A Hybrid Analytical/Experimental Modeling Approach

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Agent Fate Team at Kettering

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Project Summary

Determine the fate of an agent after it is deposited on the ground

- **Proposed Approach:** Development of a hybrid (Numerical and Experimental) method based on validated numerical algorithms with indoor and outdoor data

- **Benefits:**
  - To enhance the ability of DoD to predict in general the fate of chemical agents after they are deposited on substrates of interest
  - To provide a tool to reduce the number of required outdoor/wind tunnel experiments for the verification purpose and cost-effectiveness
  - To provide a tool for scaling indoor experiments to outdoor conditions when possible
  - To provide DoD with a tool for prediction of hazardous industrial chemicals fate
Uniqueness of Team Kettering

- Experienced in developing sophisticated and simple-to-use numerical models for widely used practical problems (Available through CPIA)
  - TDK (JANNAF Standard software for liquid rocket engine performance)
  - SPP (JANNAF Standard software for solid rocket motors)
  - VIPER (JANNAF Standard software for liquid rocket engine performance)
  - GTBL (for gun propulsion)
  - AOE (Aero-Optics) / ATHENA (Shock/Plume radiation signature – THADD Program)
  - LTCP (Two-phase flow – dense spray combustion for NASA)
Problem at Hand: Determine the fate of an agent after it is deposited on the ground

- Technology involved
  - Surface evaporation
  - Liquid transport through porous substrate
  - Evaporation within the pores
  - Vapor transport
  - Surface adsorption/reaction

- Solution proposed
  - Decouple processes
  - Model development and V & V for every process
  - Super-impose/couple all phenomena
  - Validate with outdoor data
Characteristics of the Problem at Hand

- Large Scale Problem (LSP)
- Many complex phenomena with different time and length scales are involved
- Traditional approach (No other alternative available)
  - Create a design of experiment (DOE) matrix (all variables / several levels)
  - Collect data for entries in DOE matrix
  - Use curve fits to have a generic “closed form” solution that is case dependent
  - Benefit
    - Somewhat “low risk”
  - Drawbacks
    - A priori knowledge of the end point of each curve
    - Not general enough
    - No clear path from wind tunnel experiments to outdoor situations
    - Not cost-effective
Proposed Solution – Hybrid Approach

- Development of a hybrid model based on validated numerical algorithms with indoor and outdoor data
  - Rationale
    - Marching in real time because of the nature of outdoor wind, temperature, and relative humidity variations
    - Use the model to design experiments for measuring all key transport variables that are invariant to indoor or outdoor conditions
      - Capillary pressure, permeability, effective diffusion coefficient, secondary evaporation, surface adsorption/reaction rates
    - Use the model to identify scalable groups of variable that remain invariant to indoor and outdoor data
    - Use the model to fill more entries in the design of experiment matrix (Less expensive)

- Development of a Neural Network program to predict the outcome of the DOE matrix without any prior knowledge of specific points of any curve (Superior to standard curve fit)
  - Clustering algorithm
  - Can be used with available data
Hybrid Approach - Components

Experiments
- Wind Tunnel
- Outdoor

Modeling
- Continuum
- Discrete

Off-line Outputs
- All Possible cases
- High Resolution

Suite of Models – Can be Integrated into Operational Tools
- Neural Network runs on
  - PDA
  - Wrist wearable wireless computers
Numerical Models

- Two numerical models are being developed in parallel to solve problems involving:
  - Surface evaporation
  - Liquid transport through porous substrate
  - Vapor transport – Effective diffusivity measurements
  - Evaporation within the pores – Secondary evaporation
  - Surface adsorption/reaction

- Discrete model
  - Suitable for homogeneous and non-homogeneous media
  - Cross checks the continuum model

- Continuum model
  - Suitable for all media with a known porosity or non-homogeneity
  - Suitable for scalability studies

- Neural Network as a “platform”
Agent Fate – Surface Evaporation
HD and VX on Glass – Wind Tunnel

Surface evaporation – Free or forced convection

\[ \dot{m} = \frac{\mu}{Pr} \left( F_T + C_T Re^{m_T} Pr^{n_T} \right) \ln \left[ 1 + \Lambda(T, Y_s) \right], \quad \text{model 1} \]

\[ \dot{m} = \frac{\mu}{Sc} \left( F_M + C_M Re^{m_M} Sc^{n_M} \right) \ln \left[ 1 + \Omega(Y_s) \right], \quad \text{model 2} \]

\[ \Lambda(T, Y_s) = \left( \frac{Y_s}{1-Y_s} \right)^{\xi(\Theta)} \quad \text{and} \quad \Omega(Y_s) = \left( \frac{Y_s}{1-Y_s} \right)^{\eta(\Theta)} \]

\[ \Theta = \frac{T}{T_{ref}} \quad \text{(Absolute temperatures) and} \quad Y_s = \frac{P_{vap}}{P} \]

HD \begin{cases} 
\xi(\Theta) = -57.6148 + 174.5781\Theta - 172.7751\Theta^2 + 80.40564\Theta^3 \\
\eta(\Theta) = -62.129326 + 188.072384\Theta - 186.00983\Theta^2 + 61.290737\Theta^3 
\end{cases}

VX \begin{cases} 
\xi(\Theta) = 75700.756 - 360372.25\Theta + 685421.89\Theta^2 - 651058.767\Theta^3 + 308841.05\Theta^4 - 58531.726\Theta^5 \\
\eta(\Theta) = -14981.821 + 55970.67\Theta - 78298.65\Theta^2 + 48616.52\Theta^3 - 11305.02\Theta^4 
\end{cases}

Coefficients were obtained by using some of the wind tunnel data
Agent Fate – Surface Evaporation HD on Glass – Wind Tunnel

- Used some of the data to find model coefficients
- Validation with all the data – Wind tunnel

How to estimate turbulence intensity?

Change the turbulence intensity until you get close to friction velocities measured at ECBC wind tunnel
Agent Fate – Surface Evaporation HD on Glass - Outdoor

- Validation - Outdoor

HD on Glass Czech Outdoor Trial 10-03-01
Average Drop Mass = 0.028 mg
Areal density = 160000 drops/m²
Turbulence Intensity = 1.0%

HD on Glass Czech Outdoor Trial 10-10-01
Average Drop Mass = 0.03 mg
Areal density = 160000 drops/m²
Turbulence Intensity = 1.0%
Agent Fate – Surface Evaporation
HD on Glass - Outdoor

 Validation - Outdoor

HD on Glass Czech Outdoor Trial 08-29-2002
Average Drop Mass = 0.032 mg
Areal density = 150000 drops/m²
Turbulence Intensity = 1.0%

HD on Glass Czech Outdoor Trial 09-03-2002
Average Drop Mass = 0.032 mg
Areal density = 160000 drops/m²
Turbulence Intensity = 1.0%

% Mass Left vs Time (hr)

Outdoor Data
Model 1
Model 2
Agent Fate – Surface Evaporation
HD on Glass - Outdoor

Validation - Outdoor

HD on Glass Czech Outdoor Trial 09-05-2002
Average Drop Mass = 0.04 mg
Areal density = 160000 drops/m²
Turbulence Intensity = 1.0%

Czech Outdoor Trials 09/14/2005 - Gravimetric Data
HD on Glass
Average Drop Mass: 0.027 mg
Areal Density: 656437/m²
Turbulence Intensity: 1.0%
Agent Fate – Surface Evaporation
HD on Glass - Outdoor

Validation - Outdoor

HD on Glass - Czech Outdoor Trials 6/14/06
Turbulence Intensity = 1.0%
(Automatic dissemination)
Average Drop Mass: 0.06078 mg
Areal Density: 366029/m²

HD on Glass - Czech Outdoor Trials 6/14/06
Turbulence Intensity = 1.0%
(Manual dissemination)
Average Drop Mass: 1.15 mg
Areal Density: 10000/m²

Czech Outdoor Trial 07/25/2006
HD on Glass
Average Drop Size: 1 µL
Areal Density: 10000/m²
Turbulence Intensity: 1.0%
UNCLASSIFIED

Agent Fate – Surface Evaporation
VX on Glass – Wind Tunnel

-validation – Wind tunnel (VX) – Evaporation continues in the model, but it actually stops in experiment
Identify the $\Pi$ groups - Buckingham Theorem

$$m_{\text{left}} = f \left[ t, u^*, V, r, m_{\text{initial}}, \ln(1 + B) \right]$$

Contact Angle, $\theta = g(V, r)$

$$\Pi_1 = \frac{m_{\text{left}}}{m_{\text{initial}}}, \quad \Pi_2 = tu^* \left( \frac{V}{r^2} \right)^{-1} \ln(1 + B)$$

$$\frac{m_{\text{left}}}{m_{\text{initial}}} = f \left[ tu^* \left( \frac{V}{r^2} \right)^{-1} \ln(1 + B) \right]$$
Let’s test the Π groups

For all Turbulence Intensities (0.3, 1, 2, 3, 4, 6%)
For all Velocities (0.26, 1.77, 3, 3.66, 10 m/s)
For all Droplet Sizes (0.1, 1, 5, 10, 50 μL)
For all Temperatures (15, 20, 25, 30, 35, 50, 55 °C)

Model

Experiments

Similar Solution for all the Experimental Data
Agent Fate – Surface Evaporation

Conclusions

- Developed a numerical model for HD and VX surface evaporation
- Scaled the wind tunnel data for outdoor applications
- Demonstrated that the normalized mass left is a function of the non-dimensional time
  \[ tu^* \left( \frac{V}{r^2} \right)^{-1} \ln(1+B) \] regardless of the size of the droplet
- Verified the model with outdoor data
Liquid transport in a porous substrate requires the transport properties (not a function of indoor or outdoor conditions)

- Porosity of the substrate – Can be measured
- Saturation permeability
  - Can be found by a simple experiment designed at Kettering
- Relative permeability
  - Hybrid method is used to find the generic function
- Capillary pressure
  - Have determined scalable experiment for finding the capillary pressure
Previously discussed the experimental methods for measuring porosity and saturation permeability

Porosity

<table>
<thead>
<tr>
<th>Substrate Porosity (%)</th>
<th>Tile</th>
<th>Glass Beads</th>
<th>Coarse Sand</th>
<th>Medium Sand</th>
<th>Fine Sand</th>
<th>Saudi Arabian Sand</th>
<th>Green Tea Sand</th>
<th>New Mexico Sand</th>
<th>UK Sand</th>
<th>Silica Gel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substrate Porosity (%)</td>
<td>26</td>
<td>28</td>
<td>31</td>
<td>32</td>
<td>37</td>
<td>37</td>
<td>38</td>
<td>39</td>
<td>44</td>
<td>89</td>
</tr>
</tbody>
</table>

Substrate Saturation Permeability, $K$ (m$^2$)

<table>
<thead>
<tr>
<th>Substrate Saturation Permeability, $K$ (m$^2$)</th>
<th>Tile</th>
<th>Fine Sand</th>
<th>Coarse Sand</th>
<th>Glass beads</th>
<th>UK Sand</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substrate Saturation Permeability, $K$ (m$^2$)</td>
<td>5.00 x 10$^{-14}$</td>
<td>2.30 x 10$^{-12}$</td>
<td>2.84 x 10$^{-12}$</td>
<td>4.80 x 10$^{-13}$</td>
<td>6.05 x 10$^{-12}$</td>
</tr>
</tbody>
</table>
Agent Fate
Determining Relative Permeability

Experimental Apparatus

Fine Sand + Ethylene Glycol

Experimental (for Ethylene glycol)

- **Substrate preparation**
  - Substrate: sand (100 ~ 120 g; 32.0 X 3.0 X 0.75 cm³)

- **Liquid loading**
  - Liquid: Ethylene glycol (10 mL) or Water (8 mL)

- **Spread**
  - 0 hr ~ 168 hr (7 day)

- **Cut**
  - Divided to 9 cuts (3.2 X 3.0 X 0.75 cm³)

- **Extraction**
  - With 50 mL MeOH

- **Quantification**
  - GC - FID
Agent Fate
Determining Relative Permeability

- Saturation as a function of cut $s=f(z)$, ($z$ along the channel)

Plot of Corrected 0, 6, 48, 66 and 216 hour glycol weights v. well for United Kingdom sand
Agent Fate
Determining Relative Permeability

- Saturation as a function of cut $s=f(z)$, ($z$ along the channel)

Flow Distribution (Ethylene glycol)

Relative permeability for UK sand with water
Algorithm:

- Assume a function for relative permeability, say $k_{r\ell} = s^n$
- Compare the experimental and analytical results for the function: $s=f(z)$
- Fairly good match → Function is OK
- Not a good match → Assume another function

In our case

$$k_{r\ell} = s^2$$
How can we find the capillary pressure function? Nothing in the literature for our problem

Postulate:

- Capillary pressure has the following form

\[ p_c = f(*) \frac{\sigma \cos \theta}{\sqrt{K_{sp} / \phi}} J(s_{\ell}), \]

where \( J(s_{\ell}) = 1.417(1 - s_{\ell}) - 2.120(1 - s_{\ell})^2 + 1.263(1 - s_{\ell})^3 \)

Can we find a universal function for \( f(*) \)?
Use the \( \Pi \) group approach just like the surface evaporation

- The following function is found

\[
\Pi_1 = \frac{t_{\text{ref}} \sigma K^{0.5} \mu \left( \frac{V_{\text{Initial}}}{r_{\text{Initial}}^2} \right)^2}{f(\theta, \phi)}
\]

- Test the function
Capillary Pressure Master Curve HD on Glass Beads – Model prediction

\[ 1/t^{\ast} = \text{Non-Dimensional Measured Time} / \text{Non-Dimensional Reference Time} \]

Curve Generated Using HD on a 4.6-D mm Base of Glass Beads

Non-Dimensional Reference Time: \( t_{\text{ref}} \sigma R^{0.5} / V_{\text{initial}}^{2} f_{L} \)

Initial Contact Angle, \( \theta_{\text{initial}}(^\circ) \)
Capillary Pressure Master Curve HD on UK Sand – Model prediction

$1/f(*) = \text{Non-Dimensional Measured Time/Non-Dimensional Reference Time}$

Curve Generated Using HD on a 4.6-D mm Base - UK Sand

Non-Dimensional Reference Time $= t_{ref}C_0K^{0.5}\left(\frac{r_{initial}}{V_{initial}}\right)^{2/3}r_{initial}$
Capillary Pressure Master Curve
1-2-P-D on UK Sand – Model prediction

Measurements:
- Initial contact angle
- Time for the droplet to disappear from the surface

Calculate non-dimensional measured time

Specify the general function for a specific substrate and agent
Determination of Effective Diffusivity

Run numerous experiments for a variety of

- Substrates (functionality on porosity)
- Saturation levels (by distributing inert liquid drops inside the pores) – Functionality on saturation

Measure the amount of vapor as a function of distance by using GC

Generate a “general” function
Agent Fate – Determination of the Effective Diffusivity

- One-dimensional steady-state evaporation equation
  
  \[ \dot{m} = \frac{C_1 - C_2}{R} \]
  
  Where \( R = \text{Resistance} = \frac{L}{\rho D_{\text{eff}} A} \)
  
  and \( D_{\text{eff}} = D_{\text{vap} \rightarrow \text{air}} f(\phi, s) \)

- Concentration has a linear profile

- Evaporation rate, \( \dot{m} \) can be measured on a balance (Constant at steady-state)

- \( C_1 \) and \( C_2 \) (vapor concentration) can be measured by GC

- \( D_{\text{eff}} \) can be calculated from the above equation

Exposed to a source of evaporating liquid phase.

Constant Concentration, \( P_{\text{vap}}/P = C_1 \)
Determination of the Effective Diffusivity - First Experimental Setup

Substrate: Sand
Chemical: Diethyl Malonate

Quantification by GC + Extraction

Small gap to prevent the liquid capillary effect
Determination of the Effective Diffusivity - Second Experimental Setup

Apparatus and Method 2
(sampling from the side using Micro Drop method)

Substrate: Sand
Chemical: Diethyl Malonate

Small gap to prevent the liquid capillary effect

Quantification by GC + Micro drop
Achieving Constant Evaporation Rate

Mass Loss as function of time

Rate of Mass loss ($\Delta m/\Delta t$)

Mass loss (10^{-4}g)

Rate of Mass loss (10^{-4}g/min)

time (min)
Concentration Profile in the Substrate Results for Method 1

5.5 Days Extraction

Volume (μL) vs. Depth (mm)
Concentration Profile in the Substrate Results for Method 2

**Acetonitrile**

Amount of acetonitrile in each "layer (12.5mm)" (μL)

```
y = -0.1698x + 14.044
R^2 = 0.9815
```
Effective Diffusion Coefficient as a Function of Porosity and Saturation

Saturation trial with pentane through fine sand

\[ y = -78.996x + 8.2445 \]
\[ R^2 = 0.993 \]

Concentration of Pentane (mol/m^3)

Depth of sand (m)

- 0%
- 15%
- 30%
- 45%
- 60%

Linear (0%)
Effective Diffusion Coefficient as a Function of Porosity and Saturation

Saturation trial with pentane through UK sand

Concentration of pentane (mol/m³) vs Depth of sand (m)

- 0%
- 15%
- 30%
- 45%
General function for the Effective Diffusion Coefficient

\[
\frac{D_{\text{effective}}}{D_{\text{Molecular}}} = \phi \left[ -0.5855(1 - s)^3 + 0.7591(1 - s)^2 + 0.5557(1 - s) \right]
\]

\[\phi = \text{Porosity}\]
\[s = \text{Saturation}\]
Secondary Evaporation Experimental Setup

- Inject 200 $\mu$L of Acetonitrile (liquid) in the middle
- Measure mass loss as a function of time on the balance
- Analyze the longitudinal vapor concentration as a function of time (GC micro-drop)
Secondary Evaporation Mass Left (Measured from the Balance)

Mass loss of Acetonitrile loaded from middle through fine sand

![Graph showing mass loss over time](image-url)
Secondary Evaporation - Fine Sand

Micro-Drop vapor analysis above the injection port

![Graph showing GC Area vs Port Number above with data points and linear fits for 1 hr and 2 hr.]  
- GC Area vs Port Number above
- Data points for 1 hr and 2 hr
- Linear fits for 1 hr and 2 hr

Micro-Drop vapor analysis below the injection port

![Graph showing GC Area vs Port Number Below with data points and linear fits for 1 hr and 2 hr.]  
- GC Area vs Port Number Below
- Data points for 1 hr and 2 hr
- Linear fits for 1 hr and 2 hr
Secondary Evaporation - Fine Sand

UK Sand_Port E

% MS recovered

port

A B C D E F G

2 4 6 24 28 48 72 96 120 144 168
Secondary Evaporation - Fine Sand
Secondary Evaporation - Fine Sand

Overall Methyl Salicylate Recovered (UK Sand)

Total % MS recovered

Time (hr)

2 4 6 24 28 48 72 96 120 144 168
Surface Adsorption/Reaction Inverse Gas Chromatography (IGC)

- This technique is based on traditional gas solid chromatography, but its goal is the characterization of the stationary phase rather than the separation of solutes.
- Study the adsorption capability, and adsorption strength and specificity of interaction between adsorbents and compounds in gas phase.
Inverse GC - Instrument
Inverse GC - Temperature and Flow Rate Control

**IGC System: (Varian 3400)**

temperature variation < 1 °C

**GC System: (Agilent 5890)**

temperature variation < 1 °C

**Gas flow Controller:**
Agilent® 7890A Digital flow controller
Inverse GC – Porous Substrate Column

- **Column**: Stainless steel column (170 mm in length, 4 mm in diameter) with 1 mm thickness

- **IGC Injector temperature**: 100 °C
- **IGC Column temperature**: 27~120 °C
- **GC Detector temperature**: 200 °C
- **Detector**: FID
- **Carrier gas**: N₂
- **Flow Rate**: ~ 2 mL/min
- **Loading amount**: 1 µL
**Inverse GC – Pentane Adsorption**

- **molecular formula:** $\text{CH}_3(\text{CH}_2)_3\text{CH}_3$
- **molar mass:** 72.15 g/mol
- **density:** 0.626 g/mL
- **boiling point:** 36.1 °C
- **melting point:** -129.8 °C
- **solubility in water:** 0.01 g/100 mL (20 °C)
- **vapor density:** 2.5 (air = 1.0)
- **vapor pressure:** 420 mm Hg @ 20 °C
- **viscosity:** 0.24 cPas @ 20 °C
- **evaporation Rate:** ~29 (n-Butyl Acetate = 1)
**Condition of IGC:**
Injector temperature: ~ 80 °C
Column temperature: 25~50 °C
Flow rate: ~2 mL/min
Chemical: Pentane
Loading amount: 1 uL
Substrate: wet New Mexico sand
Inverse GC – Substrates Testes

Glass bead
- porosity: 0.39
- density: 1.59 g/mL

Silica Gel (30~60 mesh)
- porosity: 0.81
- density: 0.38 g/mL

Green Tea sand
- porosity: 0.38
- density: 1.63 g/mL

New Mexico sand
- porosity: 0.39
- density: 1.59 g/mL
Retention Time as Function of Temperature for Silica Gel

Pentane Adsorption by Silica Gel (30-60 mesh)
Retention Time as Function of Temperature for Glass Beads
Retention Time as Function of Temperature for New Mexico Sand

Pentane Adsorption by New Mexico Sand

Retention Time (min)

Temperature (K)
Comparison of Pentane Adsorption by Glass Bead, New Mexico sand, Silica gel and Green Tea Sand (GC retention time vs. temperature)
Capillary Network Model
- Models the pores as a network of passages connected together
- Moves the liquid inside the pores randomly by balancing viscous, capillary pressure (Darcy’ Law), and gravitational forces
In a discrete step, all pores that satisfy capillary threshold are filled/emptied,
Capillary Network Modelling

Comparison between numerical and experimental spread on ceramic tile,

**Glycerin:**
- High viscosity
- Small imprint changes

**1,2-P-D:**
- Low viscosity
- Larger imprint changes

$t=5, 10, \text{ and } 20 \text{ min}$

$t=2, 5, 10, \text{ and } 20 \text{ min}$
Transient behavior of the secondary spread

- \( t_{sec} = 0 \) min
- \( t_{sec} = 2 \) min
- \( t_{sec} = 5 \) min
- \( t_{sec} = 10 \) min
- \( t_{sec} = 20 \) min
Discrete Model
Heterogeneous Medium – 3D
Mathematical Models - Discrete
Mathematical Models - Discrete

- Homogeneous and non-homogeneous substrates
Mathematical Model - Continuum

- Uses partial differential equations for the transport of liquid and gaseous phase with source and sink terms representing mass loss or gain by evaporation or adsorption/reaction mechanisms.
- Equations are numerically solved with explicit Runge-Kutta finite difference scheme.
Mathematical Model - Continuum

- Performed about 30 validations using different substrates and simulants
- Performed 100’s of validations using different substrates and other chemicals (Glycerin, 1-2 Propanediol, Caster oil, water, etc.)
Comparison of Time that takes for a drop to disappear from the surface – Validity of proposed Master curve for capillary pressure function. Substrate: UK Sand

<table>
<thead>
<tr>
<th>Substance</th>
<th>Experiment (Time, sec)</th>
<th>Model (Time, sec.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2-P-D</td>
<td>1.45</td>
<td>1.50</td>
</tr>
<tr>
<td>Castor Oil</td>
<td>27.50</td>
<td>28.80</td>
</tr>
<tr>
<td>Glycerin</td>
<td>12.30</td>
<td>11.70</td>
</tr>
<tr>
<td>VX</td>
<td>1.50</td>
<td>1.40</td>
</tr>
<tr>
<td>HD</td>
<td>0.90</td>
<td>0.85</td>
</tr>
</tbody>
</table>
HD on UK Sand

2 μL HD drop on UK Sand
Time for droplet disappearance = 1.5 sec.

Model

Courtesy of Dr. Terrence D’Onofrio at ECBC
VX on UK Sand

Model

Courtesy of Dr. Terrence D’Onofrio at ECBC
VX Spread into UK Sand Model/Experiment Comparison

a. Top-down image of VX on sand at 250 min. The white scale-bar represents 5 mm. The perimeter of the wetted region has been outlined for clarity. The image is shown at the same scale as the model in c.

b. Top-down rendering of model results for VX on sand spread at 250 min. Colors indicate saturation values. Model is plotted at the same scale as the experimental data shown in a.

c. Replicate spread experiments for VX on sand. Note that the data for each experiment is relatively smooth and self-consistent compared to the test-to-test variance.

d. Compilation plot comparing the experimental measurements to the numerical solutions. Closed circles (○) show the average response (n=11) of the experimental results and error bars show the 95% confidence limit. Open squares (□) and triangles (△) indicate the model predictions for the area, based on saturation values of 1% and 2% respectively.
Agreement between the experimental- and numerical- results for VX penetration into sand. Plot of depth measurements versus the square-root of time for 6 μL VX on medium-grain sand. The black line represents the penetration predicted by the model. Blue lines represent the power law fit of the experimental data.
Mathematical Model - Continuum

- Uses partial differential equations for the transport of liquid and gaseous phase with source and sink terms representing mass loss or gain by evaporation or adsorption/reaction mechanisms.
Mathematical Model – Continuum HD on UK Sand

Droplets of different sizes
Dynamics of the spread

0.095 sec

2.7 sec
Neural Network as a Platform for Hybrid Modeling Integration

- Neural network (NN) program is trained by a database of experimental and analytical data
- NN program can perform piece-wise fit based on the resolution of data provided
- NN program is based on the ™LabView Software
- NN is prepared off-line
- NN can be installed on PDA’s or wrist wearable wireless computers
- NN generates an output based on the provided input and the type of training
VX on Asphalt – Czech Data

Testing

Prediction

Tip: Click on test file to see waveform after clicking on test button below

Percentage drop at a selected time

Estimated Signal  Desired Signal

1  82.2

1  63

Tip: Click on test file to see waveform after clicking on test button below

Percentage drop at a selected time

Estimated Signal  Desired Signal

1  85.5

1  100
VX on Concrete – Czech Data

Testing

Prediction
VX on Grass – Czech Data

Testing

Output at user selectable time unit
Tip: Click on test file to see waveform after clicking on test button below

Percentage drop at a selected time

Estimated Signal Desired Signal
1 74.4 1 71.9

Prediction

Output at user selectable time unit
Tip: Click on test file to see waveform after clicking on test button below

Percentage drop at a selected time

Estimated Signal Desired Signal
1 71.9 1 100
VX on Sand – Czech Data

Testing

Prediction

Tip: Click on test file to see waveform after clicking on test button below

Percentage drop at a selected time

Estimated Signal

Desired Signal

Tip: Click on test file to see waveform after clicking on test button below

Percentage drop at a selected time

Estimated Signal

Desired Signal
HD on UK Sand – Neural Network Prediction - 1 µL, 15 °C, 0.25 m/s Wind
HD on UK Sand – Neural Network Prediction - 6 µL, 35 °C, 1.77 m/s Wind
Conclusions

- The proposed hybrid approach is a viable tool to solve any complex problem
- Experimental and modelling efforts are progressing in parallel and assisting each other
- Scaling of experiments is possible within the context of the problem in hand
- Modelling can be used effectively to design and maximize the outcome of experiments
- Experiments are a necessary part of modelling effort
- Two liquid model can be added for decontamination analysis
Acknowledgements

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