

SUPPLEMENTAL INFORMATION:

Soil Contamination by Environmentally Persistent
Free Radicals and Dioxins Following Train
Derailment in East Palestine, OH

Text S1:

EPR spectroscopy uses electromagnetic radiation to excite unpaired electrons, allowing for their detection. EPR spectroscopy was chosen for its sensitivity and specificity in detecting and quantifying the presence of EPFRs, providing detailed insights into their concentration and types. Radical concentrations are often expressed in terms of radical spins/g, which can be described as the molecules of free radicals per gram of total sample. Information about the location of the free radical within the matrix (carbon-centered, oxygen-centered, etc.) is provided by the measured g-value, which is based on the interaction between the unpaired electron and the structure of the molecule.

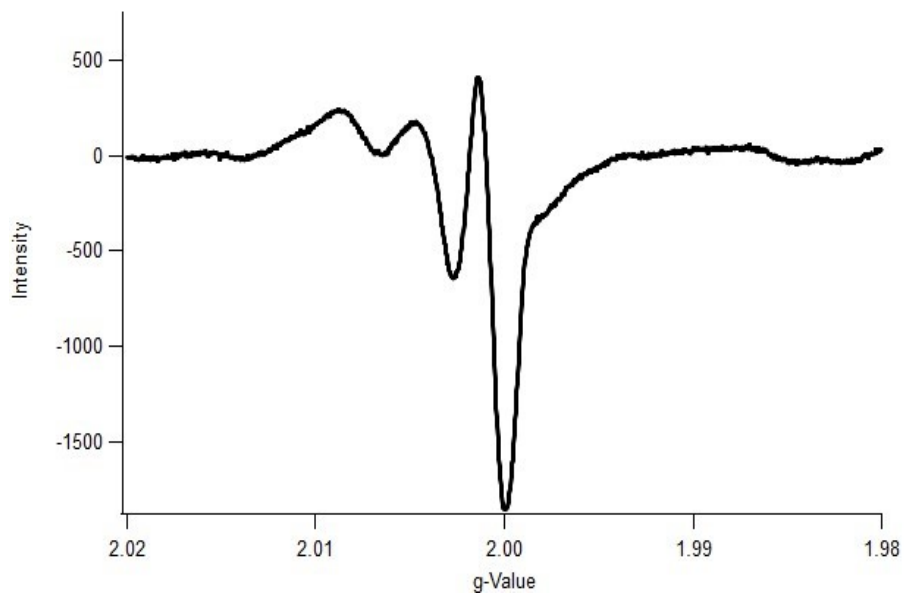


Figure S2: Electron paramagnetic resonance spectrum illustrating the complex radical signal observed on the East Palestine soil samples

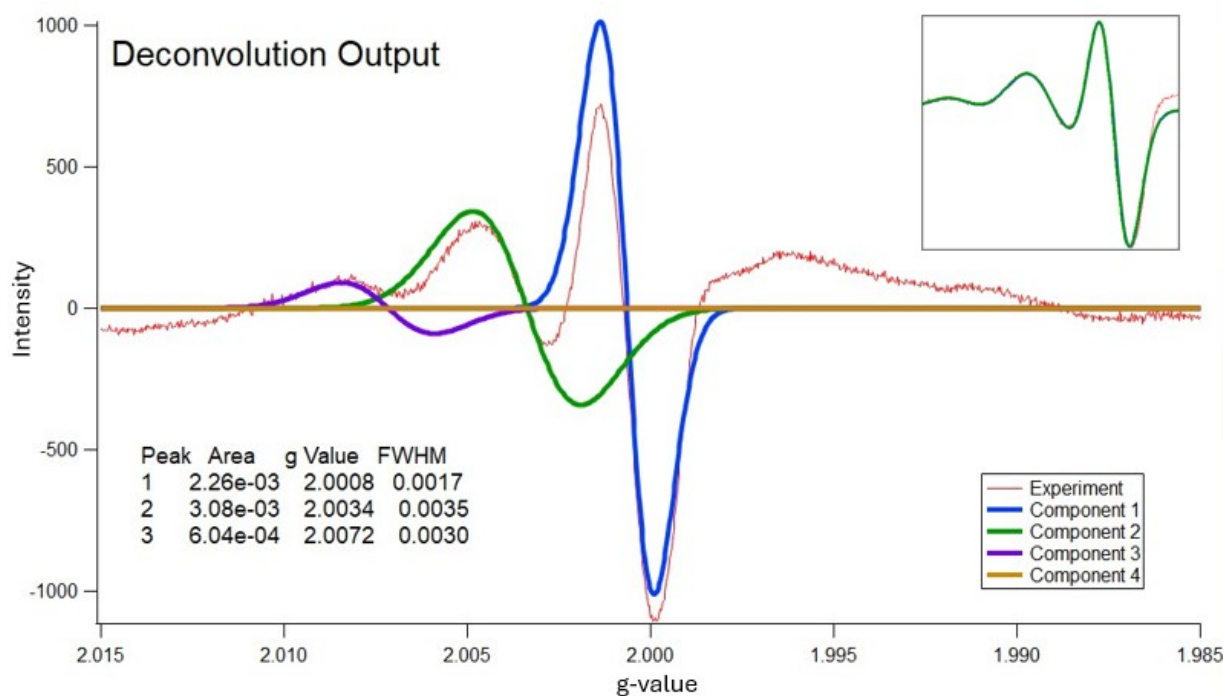
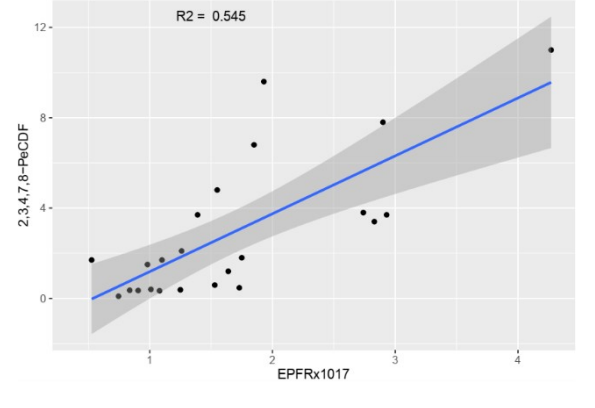
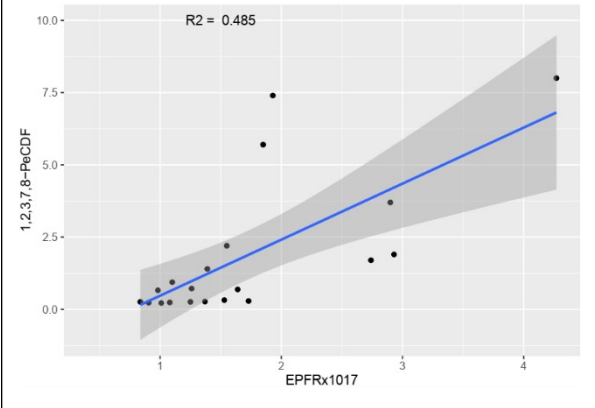
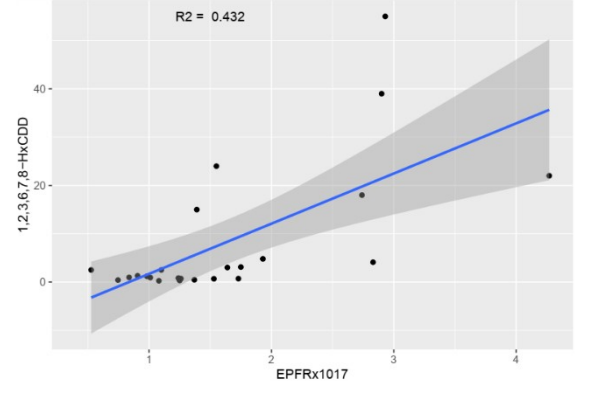
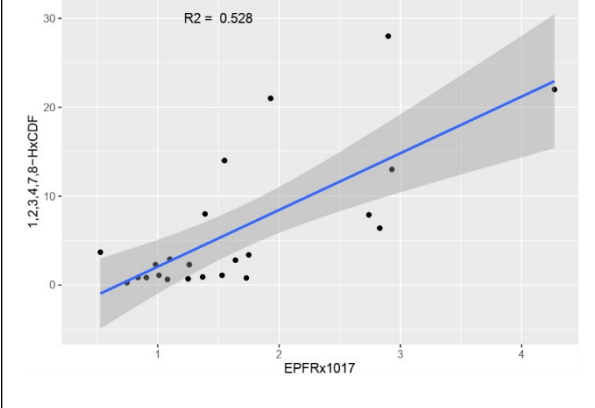
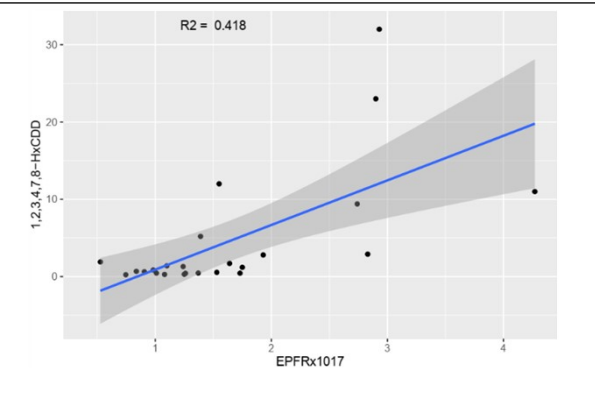
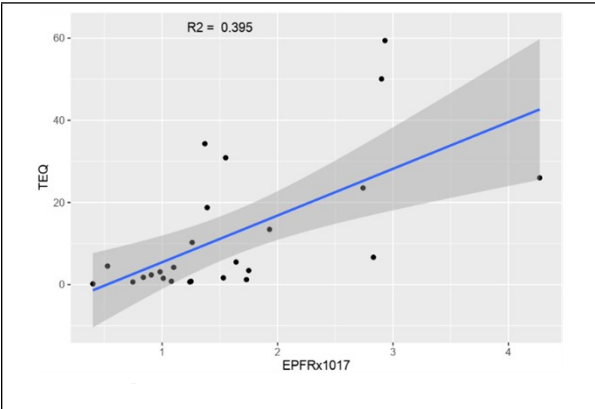


Figure S3: Output of deconvolution macro used to analyze the complex EPFR spectra observed in the dataset. Inset shows overall fit of the illustrated individual components.

Table S4: Dioxin/Furan TEQ values for urban/suburban soils adapted from Urban et al. Values for samples collected in this work are included in the bold italicized portion of the table. NR denotes a value not reported in the source work.

Source	Source Data Available	Mean TEQ (pg/g)	Median TEQ (pg/g)	Minimum TEQ (pg/g)	Maximum TEQ (pg/g)
<i>East Palestine Sampling (LSU/KSU, 2023)</i>	<i>YES</i>	<i>15.8</i>	<i>4.5</i>	<i>0.2</i>	<i>88.2</i>
USEPA Midwest Soil Screening Survey (USEPA, 1985)	YES	TCDD-only: 56.6 All congeners: 51.2	TCDD-only: 28.0 All congeners: 48.4	TCDD-only: 3.0 All congeners: 4.1	TCDD-only: 170.0 All congeners: 112.0
USEPA Columbus, Ohio (USEPA, 1996)	YES	20.2	9.2	3.0	64.0
Washington State Department of Ecology study (WDE, 2011b)	YES	19.2	12.0	1.7	120
Denver, CO soil survey (USEPA, 2002)	YES	13.1	4.4	0.2	145.7
Midwest and Ontario Soil Survey (Birmingham, 1990)	NO	9.4	1.2	0.1	78.5
University of Michigan Dioxin Exposure Study (Demond et al., 2008)	NO	6.9	3.6	0.4	186.2

(surface soil)					
TCEQ Texas Soil Survey (TCEQ, 1997)	YES	6.7	6.7	6.2	7.2
Washington State Department of Ecology study (WDE, 2010)	YES	4.2	2.0	0.7	21.0
USEPA Midwest Soil Screening Survey – Henry, IL and Middleton, OH (USEPA, 1985)	YES	TCDD-only: 2.0 All congeners: 4.1	TCDD-only: 2.0 All congeners: 3.3	TCDD-only: 1.0 All congeners: 2.2	TCDD-only:5.0 All congeners: 7.6
NIH campus soil survey in Bethesda, MD (NIH, 19950)	NO	2.2	NR	NR	NR
Survey of Midwestern and Mid-Atlantic Cities (Nestrick et al., 1986)	YES	2.2	0.9	0.2	9.4
University of Utah (RMCOEH, undated)	NO	1.3	0.9	0.3	4.5



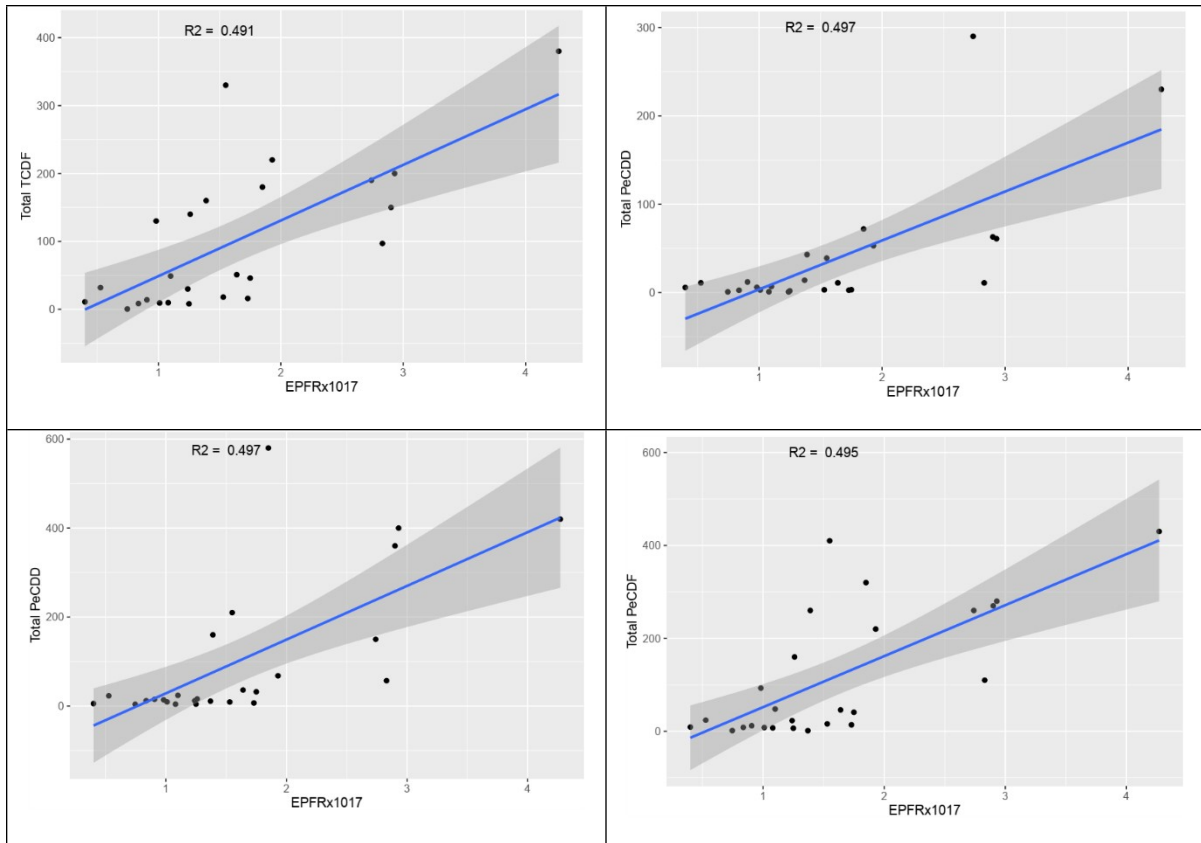


Figure S5: Statistically significant relationships of dioxin aggregate values or congeners with EPFRs ($\times 10^{17}$).

Table S6. Linear regression output with no outlier removed comparing EPFR concentrations (independent variable) to various chemical parameters (dependent variable)

Dependent Variable	Slope	p-Value	Correlation	Adjusted R ²	Outlier Removed
TEQ	8.727	0.015	0.465	0.185	No
1.2.3.4.6.7.8-HpCDD	134.580	0.098	0.325	0.070	No
1.2.3.4.6.7.8-HpCDF	29.650	0.161	0.278	0.040	No
1.2.3.4.7.8.9-HpCDF	2.126	0.134	0.308	0.055	No
1.2.3.4.7.8-HxCDD	3.492	0.063	0.369	0.101	No
1.2.3.4.7.8-HxCDF	4.212	0.033	0.428	0.148	No
1.2.3.6.7.8-HxCDD	6.506	0.097	0.332	0.073	No
1.2.3.6.7.8-HxCDF	4.253	0.010	0.503	0.220	No
1.2.3.7.8.9-HxCDD	8.054	0.055	0.381	0.110	No
1.2.3.7.8-PeCDD	2.296	0.018	0.479	0.195	No
1.2.3.7.8-PeCDF	1.939	0.001	0.696	0.456	No
2.3.4.7.8-PeCDF	1.958	0.000	0.723	0.501	No
2.3.7.8-TCDD	1.643	0.000	0.903	0.800	No
2.3.7.8-TCDF	-4.278	0.729	0.076	-0.040	No
OCDD	843.400	0.161	0.277	0.040	No
OCDF	52.880	0.210	0.249	0.025	No
Total.HpCDD	274.923	0.069	0.355	0.091	No
Total.HpCDF	64.480	0.249	0.230	0.015	No
Total.HxCDD	70.470	0.005	0.520	0.241	No
Total.HxCDF	109.390	0.008	0.498	0.218	No
Total.PeCDD	20.410	0.749	0.065	-0.036	No
Total.PeCDF	129.180	0.000	0.831	0.678	No
Total.TCDD	17.181	0.003	0.556	0.281	No
Total.TCDF	73.980	0.000	0.759	0.559	No
TOC	1.087	0.000	0.700	0.470	No
B	1.130	0.058	0.370	0.102	No
Ca	14843.00	0.000	0.723	0.504	No
Cu	8.538	0.001	0.615	0.353	No

Fe	1046.000	0.348	0.188	-0.003	No
K	-122.340	0.227	0.240	0.020	No
Mg	529.200	0.146	0.288	0.046	No
Mn	197.900	0.055	0.373	0.105	No
Na	46.952	0.000	0.813	0.647	No
P	43.550	0.359	0.184	-0.005	No
S	223.850	0.000	0.733	0.518	No
Zn	48.630	0.000	0.797	0.621	No

Table S7: EPFR analysis results for the 10 agricultural samples collected prior to derailment ~10 miles from downtown East Palestine

Sample ID	Radical Concentration (spins/g)	Organic Radical g-value	Distance from Derailment Site (mi.)
1 Deep	1.34E+17	2.0034	10
1 Shallow	1.2E+17	2.0034	10
2 Deep	1.07E+17	2.0031	10
2 Shallow	1.38E+17	2.0033	10
3 Deep	1.06E+17	2.0031	10
3 Shallow	1.33E+17	2.0031	10
4 Deep	9.32E+16	2.0035	10
4 Shallow	8.22E+16	2.0032	10
5 Deep	1.04E+17	2.0035	10
5 Shallow	8.23E+16	2.0034	10

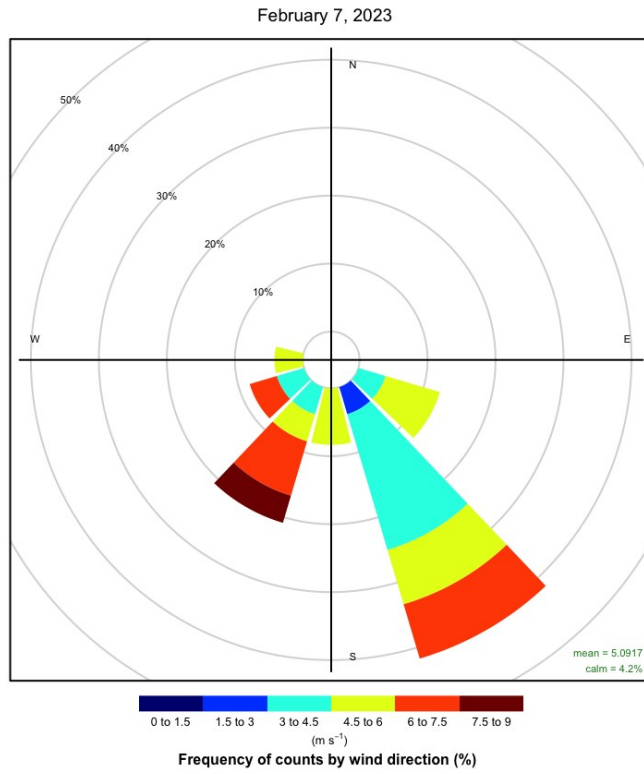
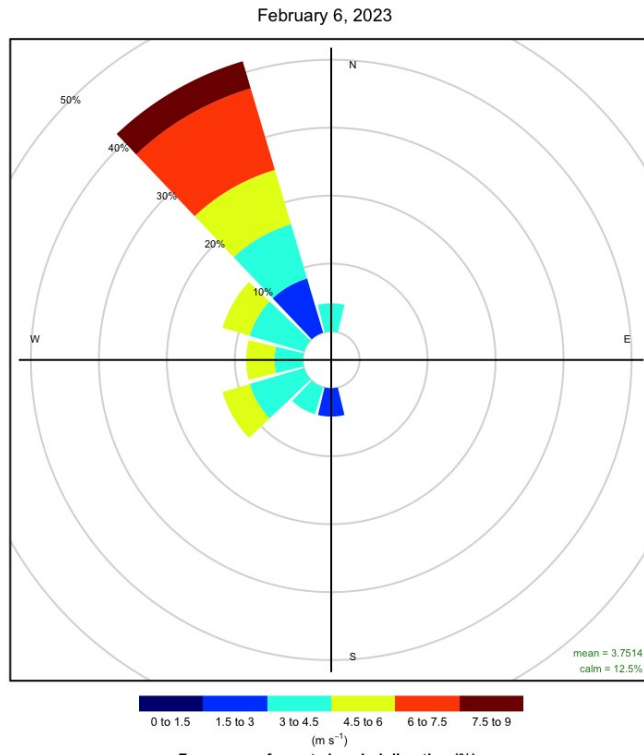


Figure S8: Wind roses for February 6 and 7, 2023, during the controlled burn.

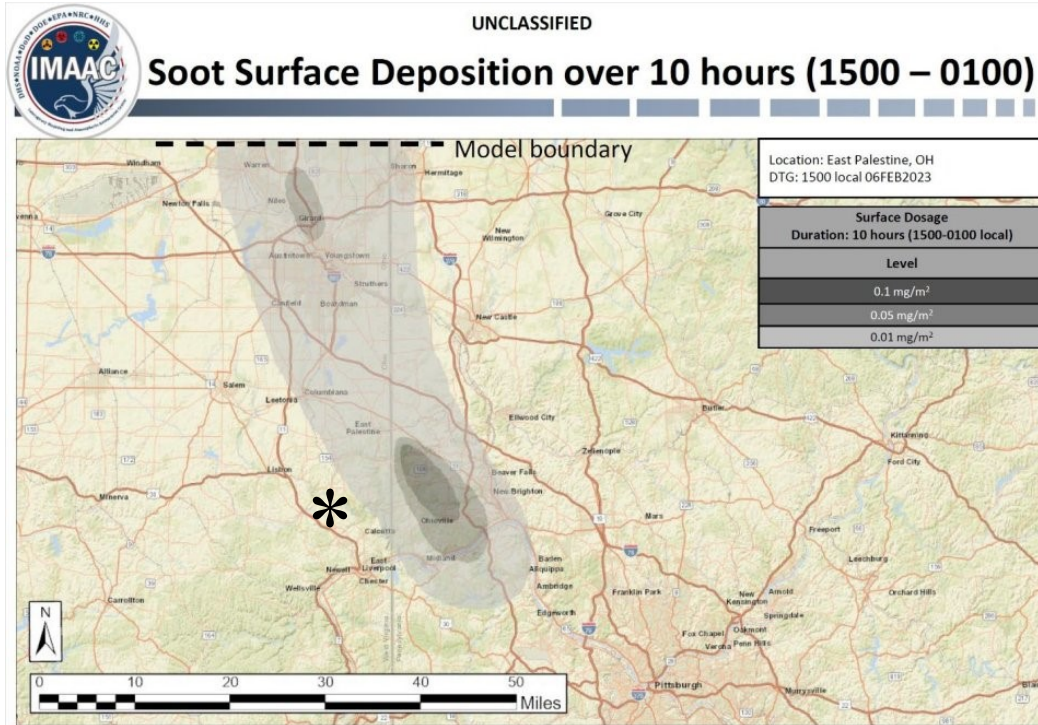


Figure S9: Interagency Modeling and Atmospheric Assessment Center model illustrating the soot deposition over 10 hours resulting from the vented burn at the derailment site. East Palestine indicated by asterisk.