Characterizing Hazard Mitigation Efficacy for Different Agent Distributions

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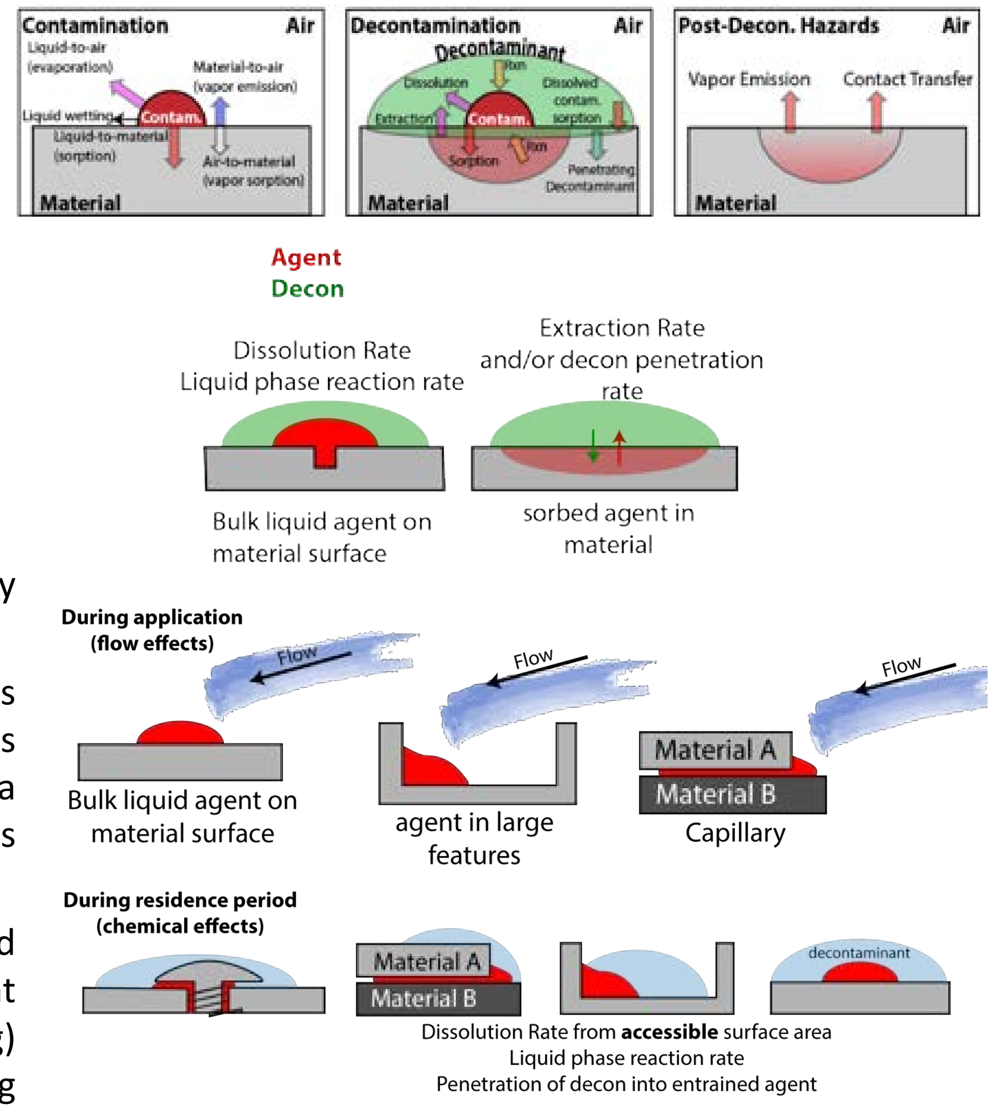
Motivation

- Hazards result from how agent retained by materials produce vapor emission or contact transfer
- The ability to remove agent from a material is dependent on the distribution of the agent on or in the material including
  - Absorbed in bulk layers
  - Adhered to surface
  - Entrained in capillary networks
- Agent distributions are affected by different rate limiting mechanisms
- For capillary entrainment large features may behave similar to flat panel but as feature size decreases there is a transition where small features significantly influence performance
- Agent distributions may be affected differently during decontaminant application process (shear and mixing) vs dissolution and reaction during decontamination residence periods



- Testing for decontamination efficacy must rely on materials-level, lab-scale tests. Therefore, specific agent distributions are created in laboratory testing to isolate and characterize the mechanisms of removal.
- The ability to bridge the gap from laboratory to field use depends on accounting for how these mechanisms contribute to removing the agent from each distribution
- New laboratory methods are presented that explore how to generate specific agent distributions, to characterize decontamination efficacy, and to evaluate how these different distributions contribute to personnel exposure

Liquid Decon Attribute	Effect
Reactivity	Ability to destroy agent, often must be dissolved first
Dissolution	Ability to dissolve agent / thickened agent
Material penetration	Ability of the decontaminant to penetrate into the material
Wettability	Ability to wet the material surfaces to interact with contaminants
Flow (sag) resistance	Ability to stay where applied
Shear flow displacement	Ability to access and remove agent from materials and in capillary recesses
Volatility	Ability to not evaporate maintain 'wetted' areas

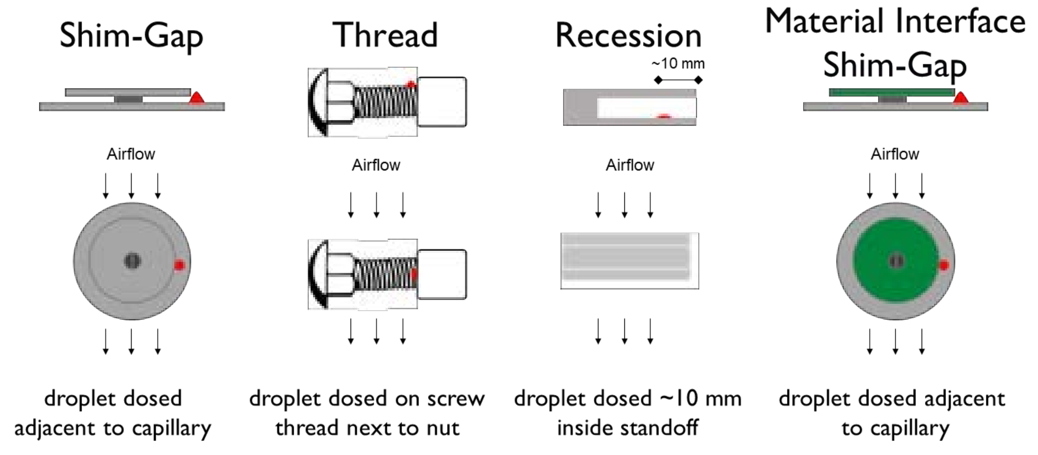
- Different **decon attributes** are required to enable decontamination depending on the agent distributions
- Specific test configurations from liquid phase reactors to different material configurations are required to characterize various decon attributes
- This work focuses on capillary entrained agent

The approach to better decontamination may not be faster direct chemical reaction, but rather addressing other rate-limiting mechanisms or decon attributes that preclude the chemical reaction

Capillary Entrainment

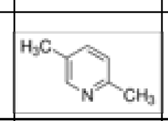
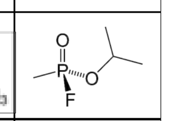
Capillary Features

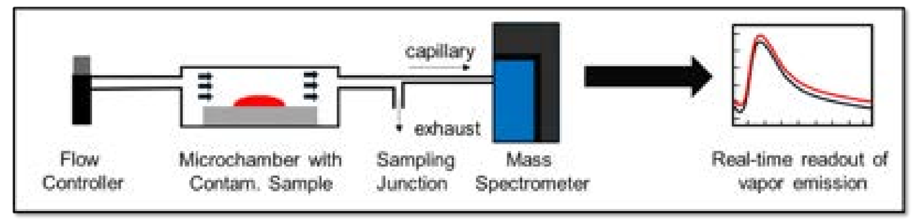
- Traditional material evaluations have focused on flat materials for testing
- Multiple types of capillary features identified and tested
- The shim-gap configuration enables a tunable size (0.025-1.5 mm) capillary gap
- Materials investigated included steel and a polyurethane coating



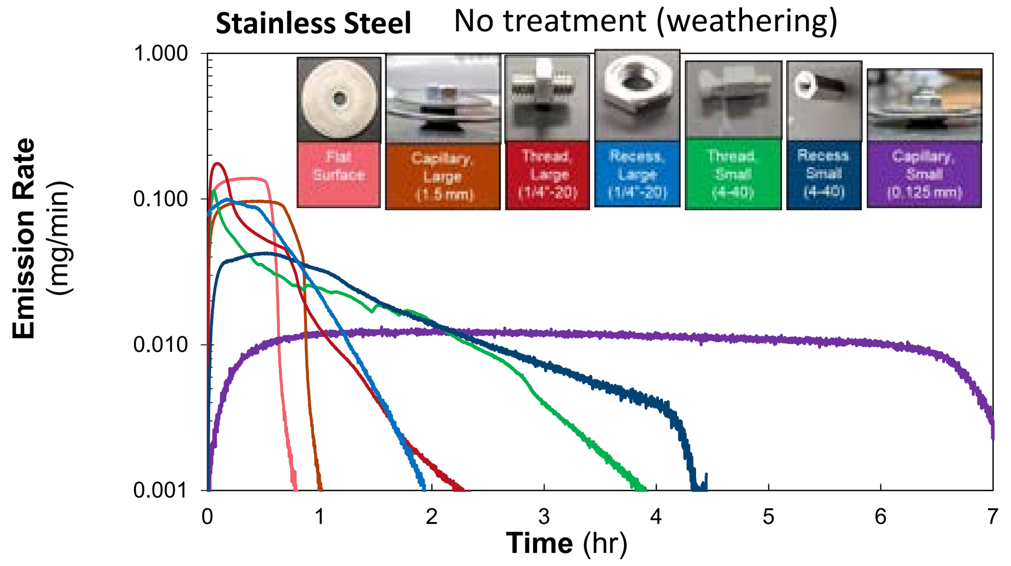
Experimental

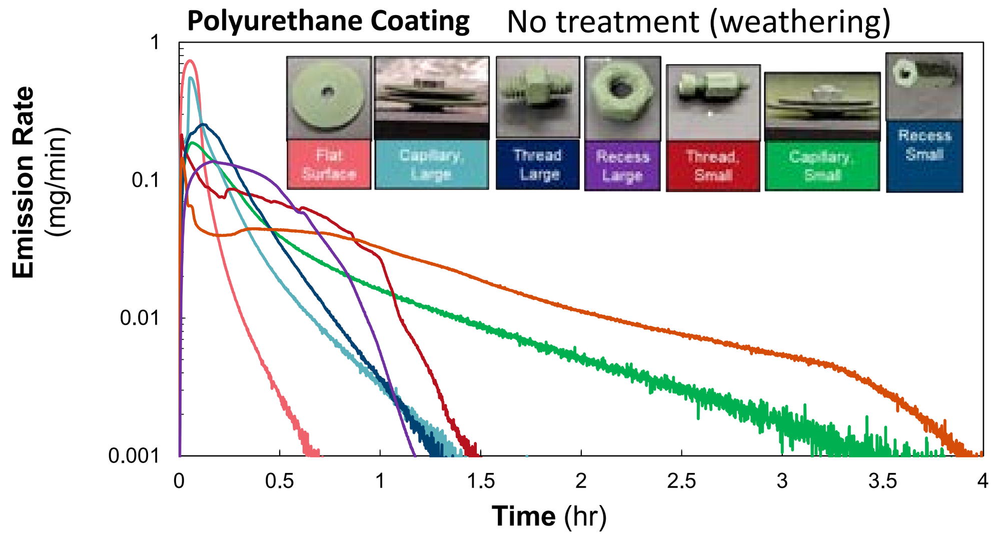
- 2, 5 Lutidine used as volatile agent simulant applied as 5 µL droplets, contamination duration of 5 min
- Samples placed in microchamber with MFC regulated N_2 air flow
- MKS Cirrus 3-XDa atmospheric pressure quadrupole mass spectrometer sampled air stream to determine emission rate
- Capillary features tested with no treatment and a water rinse to evaluate effect of a mild treatment process
- Water rinse treatment with simulant provided an idealized test bed to look at simple interactions and focus on capillary entrainment agent distributions without reactivity and other interactions

		2,5- Lutidine	GB (Sarin)
	Chemical Structure		
Vapor Emission	Boiling Point	144° C	147° C
	Vapor Pressure	2.4 Torr	2.5 Torr
Liquid Spreading	Surface Tension	30 dyn/cm	26 dyn/cm



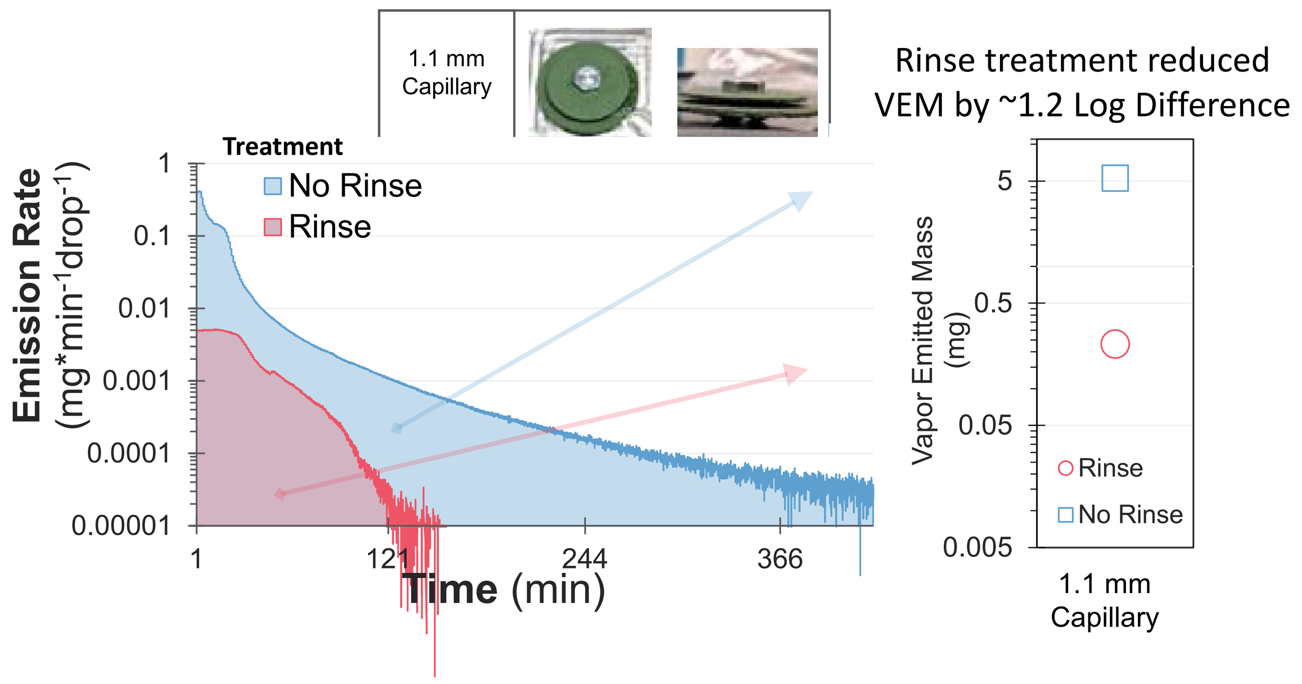
Results





- For the 'no treatment' case, all applied chemical was emitted over experiment duration
- Capillary features exhibit reduced source term *magnitude* and extend *duration*
- Across capillary types (shim-gap, threads, recession) the smaller the feature, the more the source term differs from flat panel

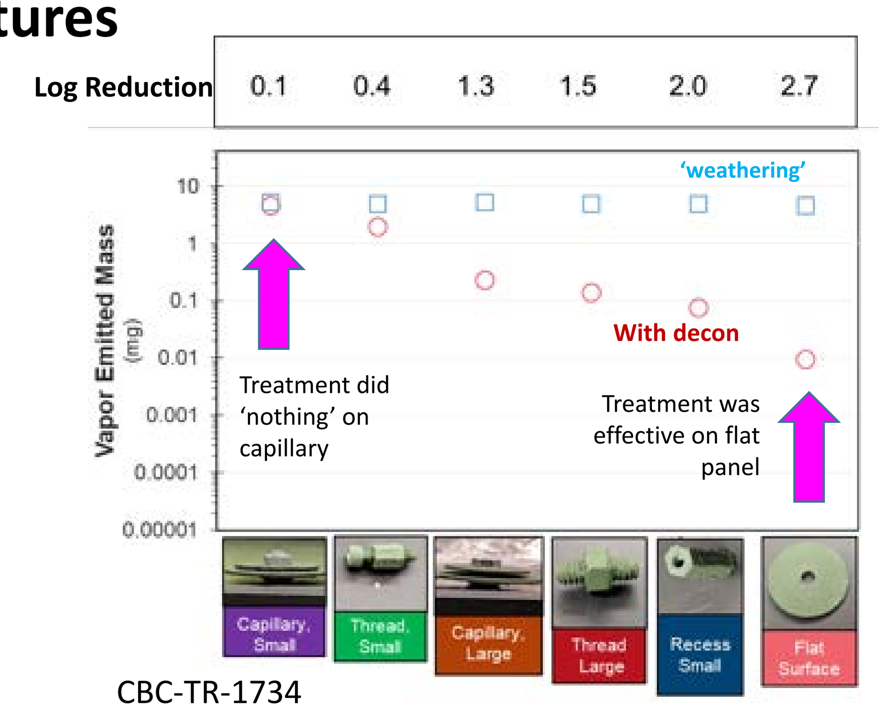
Effect of Decontamination on Capillary Features: Water Rinse Treatment



- Water rinse used as a simple decontamination treatment
- **Vapor Emitted Mass (VEM):** time integral of emission rate that captures total vapor that could result in exposure to personnel
- Treatment reduced source term magnitude, duration, and total VEM

Efficacy Across Features

- Current decontaminant performance test methodologies focus on flat horizontal materials for efficacy testing which show 'good efficacy' as indicated by log reduction in VEM on flat panels
- Water rinse is demonstrated to remove the contaminant from flat panels (2.7 log reduction) but has decreasing performance as capillary features become smaller
- As feature size decreases:
  - Capillary pressure and contaminant entrainment increase
  - Flow restriction by small features seems to inhibit decontaminant access
- Capillary feature type seems to be less influential than feature size
- Data suggests that decontamination of capillary features includes mechanisms associated with flow restrictions that are not observed on flat panel testing
- Use of capillary feature materials enables the characterization and optimization of hazard mitigation technologies to remove this type of agent distribution



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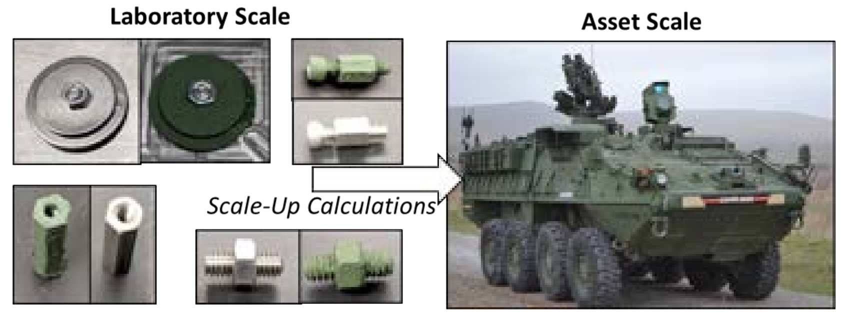
Laboratory Panels to Full-Scale Asset: Significance of Capillary Features

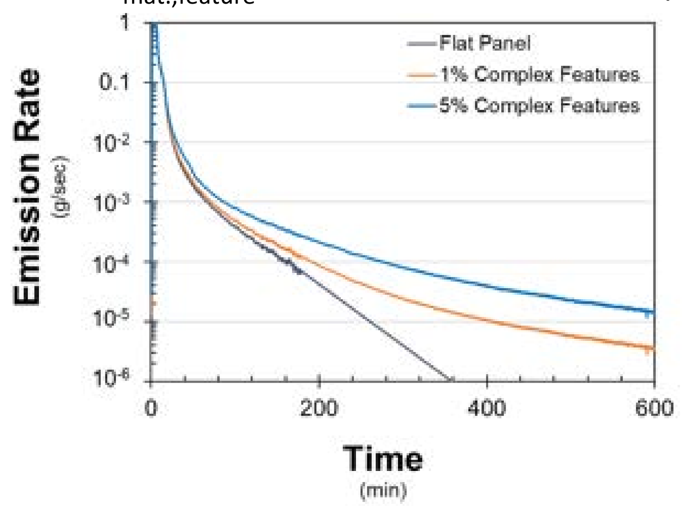
- **Question**: how much do capillary features contribute to personnel exposure?
- Lab data is used to represent full-scale assets by scaling the number of droplets that would occur on the asset
- Assume variable capillary contamination from 0-5%, how significant are capillary sources to total asset emission?

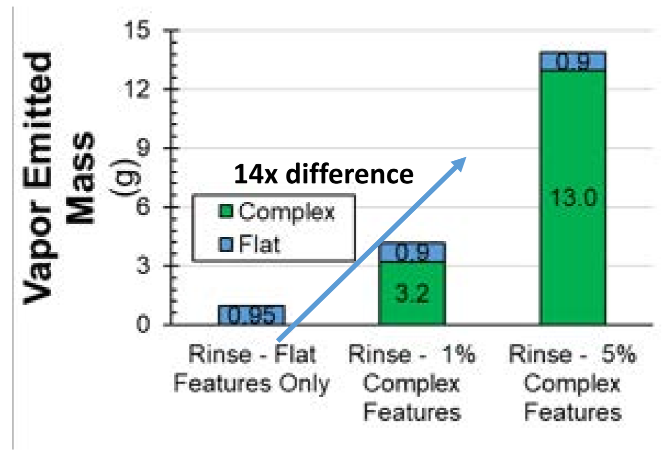


$$E_{asset} = \sum n_{drops} R_{mat.,feature}$$

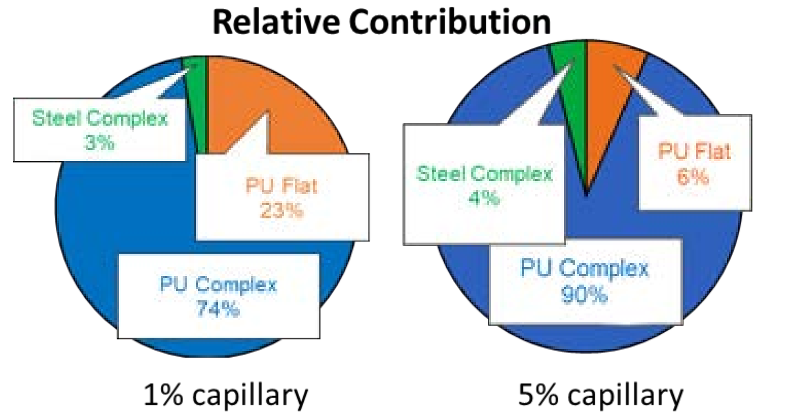
E_{asset} = total emission rate from asset (mg min^{-1})
N_{drops} = number of drops on this material/feature (drops)
$R_{mat.,feature}$ = material emission rate (mg min^{-1} drop^{-1})

Capillaries may be vital to include in testing and technology optimization
Using only flat panel materials may significantly overestimate actual technology performance on real assets





Relative Contribution



- Inclusion of capillary features in asset emission rate influenced total VEM by a factor of 14
- Small number of capillaries significantly influenced magnitude of total vapor hazard
- Relative contribution of each feature type to total asset VEM was evaluated
- Use of capillary feature panels enables characterization and optimization of technologies to address this type of agent distribution, which can significantly contribute to personnel exposure

Conclusions

- Hazard mitigation technology efficacy is influenced by how the technology can access the contaminant distribution and the associated rate limiting processes
- Removal of capillary entrained contaminant may require different mechanisms for contaminant removal
- Factors that influence agent distribution and rate limiting processes can significantly influence hazard mitigation efficacy/performance
- Laboratory testing and technology optimization should generate representative contaminant distributions and consider the relevant rate limiting processes for accurate results

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