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# Near-Field Air Modeling Tools for Potential Hazardous Material Releases from Battery Energy Storage System Fires

***Environmental Aspects of Fueled Distributed Generation and Energy Storage***

## 1. Introduction

This document was prepared to assist in selecting appropriate air modeling tools to address potential hazardous material releases resulting from stationary battery energy storage system fires. EPRI reviewed a large number of candidate modeling tools and evaluated them based on a number of criteria: (1) suitability for near-field dispersion modeling (within a few kilometers of the source or less), (2) low or moderate computing resource requirements, and (3) public availability with accessible user's guides.

Based on the material reviewed and the above criteria, EPRI found three models that have the most potential for this application: SCICHEM, the Process Hazard Analysis Software (Phast), and SAFER/TRACE. SCIPUFF, the transport component of SCICHEM, is the basis for the government Hazard Prediction and Assessment Capability Joint Effects Model (HPAC/JEM) emergency release models. The SCICHEM model allows for the potential chemistry of pollutants to be accounted for as well as the impact of terrain and nearby structures on the dispersion gradient. Phast is a comprehensive proprietary model from DNV-GL that is used to analyze accidental chemical releases. SAFER/TRACE is a proprietary modified version of the TRACE model that was designed to evaluate the environmental impacts of toxic chemical spills. Of these three, SCICHEM is the only one that is publicly available, and thus the only one that met all three criteria listed above.

In the following section, the battery fire air modeling problem is briefly described. An overview of each model considered for this application is provided in Section 3, with material synthesized from several websites, user's guides, and/or published articles. Section 4 contains brief summaries of additional, commonly used dispersion modeling tools that would be appropriate for applications with less restrictive criteria (e.g., larger-scale dispersion modeling, more compute-intensive models, not publicly available). Our recommendations for future work are provided in Section 5. Table 1 shows the models discussed below and some key attributes for each. The first entry in the table is a description of an ideal tool that would cover all attributes needed to model the desired scenarios in this application.

*Table 1. Model Attributes Overview*

| Model | Dense Gas | Buoyant Plume | Chem-istry | Terrain Impacts* | Buildings | Spatial Scale | Setup Effort | Run Time | Public |
|---|---|---|---|---|---|---|---|---|---|
| *IDEAL MODEL* | *Yes* | *Yes* | *Yes* | *Yes* | *Yes* | *Local* | *Easy* | *Fast* | *Yes* |
| ADMS-5 | Yes | Yes | Yes | Yes | Yes | Local-Regional | TBD | TBD | Licensed |
| AERMOD | No | Yes | No | Yes | Yes | Local | Easy | Fast | Yes |
| CALPUFF | No | Yes | Yes | Yes | Yes | Local-Regional | Medium | Moderate | Yes |
| CAMEO/ALOHA | Yes | No | Yes | No | No | Local | Easy | Fast | Yes |
| CMAQ | No | Yes | Yes | Yes | No | Regional-Global | Hard | Slow | Yes |
| CTDMPLUS | No | Yes | No | Yes | No | Local | Easy | Fast | Yes |
| FLEXPART | No | Yes | No | Yes | No | Regional | Easy | Fast | Yes |
| HPAC/JEM | Yes | Yes | Yes | Yes | Yes | Local-Regional | Medium | Fast | No |
| HYSPLIT | No | Yes | No | Yes | No | Local-Regional | Easy | Fast | Yes |
| Offshore and Coastal Dispersion Model | No | Yes | No | Yes | No | Local-Regional | Easy | Fast | Yes |
| Phast | Yes | Yes | No | No[+] | Yes[@] | Local-Regional | Medium | Fast | Licensed |
| SAFER/TRACE | Yes | Yes | Yes | No[+] | TBD | Local | Easy | TBD | Licensed |
| QUIC-Plume LPDM | Yes | Yes | Yes | Yes | TBD | Local | Easy | Fast | No |
| SCICHEM | Yes | Yes | Yes | Yes | Yes | Local-Regional | Medium | Moderate | Yes |
| STILT | No | Yes | Yes | Yes | No | Regional | Easy | Fast | Yes |
| WRF-Chem | No | Yes | Yes | Yes | No | Local-Regional | Medium | Moderate | Yes |
| WRF-Fire | No | Yes | Yes | Yes | No | Local-Regional | Medium | Moderate | Yes |

"TBD" means we were not able to evaluate this aspect of the model based on public information or due to the need for license fees to access the model.
*Terrain Impacts refers to the ability of the model to account for anything beyond flat surfaces.
[+]Phast and SAFER/TRACE account for different terrain by changing the roughness length only.
[@]Phast incorporates a building downwash model for the point of release, but cannot account for buildings that are downstream of the release

## 2. Description of the Battery Fire Dispersion Modeling Problem

Large format lithium-ion batteries, often deployed in storage containers for utility-scale applications, can be used to store produced electricity for later periods. However, during abnormal conditions, these batteries have the possibility to undergo thermal runaway (Electric Power Research Institute, 2018, 2019c) and might release flammable and toxic gases that then combust, leading to battery fires (DNV GL, 2020). The concern of this project is to identify modeling tools that can be used to simulate the release and dispersion of gases from these battery fire incidents both for planning purposes (such as what might be required for facility permitting) and for emergency response. For emergency response actions that could occur in near-real time, computationally fast models that require little input data are preferred. The scale of the dispersion scenario is on

the order of a few kilometers downwind of the source or less, including areas occupied by facility personnel, firefighters, and surrounding neighborhoods.

Battery fires generally have three phases. In the first, pre-combustion or incipient phase, a large amount of gas is released from the batteries for a period of seconds (one battery cell) to minutes (one module). This pre-combustion phase has the highest total gas release rate. Even if ventilated from a container, the gases released may not be well-mixed with air, and so the density of the released gases needs to be accounted for. This would require a model that handles dense gas plumes and industrial applications. In the second, combustion phase, the gases ignite, leading to an explosion and battery fire. The combustion removes a large amount of the gases released, and the process of burning mixes them with air such that dense gas effects can be neglected, but the buoyancy of the hot smoke needs to be accounted for. This requires a model that can account for buoyant plumes, such as a smokestack or plume/puff model. In the final, suppression phase, water and/or chemical agents are used by firefighters to stop the combustion, but the heat release from the batteries continues; again buoyant plume models are required. In this phase the gas emission rates are lower than in the first phase, but are not removed by combustion and the exposure of firefighters near the source becomes a concern. In this phase, dense gas and buoyancy may both need to be incorporated.

To simulate the battery fire dispersion described above, a number of meteorological and chemical variables are required. Depending on the sophistication of the model used, these include:

- Wind speed and direction
- Temperature
- Humidity
- Stability or turbulence profiles
- Chemical characteristics (e.g., species emission factors, chemical mechanisms, thermodynamic properties)
- Explosion parameters (e.g., estimates of heat release rate and total released heat)

Additionally, some models take four-dimensional data whereas others use instantaneous profiles or single-point observations. Other models can use either source of meteorological observations depending on what is available. In Sections 3 and 4, the meteorological input for each model is discussed when relevant to meeting the criteria set in Section 1.

# 3. Detailed Model Descriptions for Suitable Modeling Tools

## 3.1 SCICHEM

SCICHEM refers to the reactive version of the Second-order Closure Integrated PUFF (SCIPUFF) model (Electric Power Research Institute, 2019a). SCIPUFF is a Lagrangian transport and diffusion model used for the simulation of atmospheric dispersion. Three dimensional puffs are used to represent the concentration field in the Gaussian puff method (Wendell et al., 1976), which is implemented in SCIPUFF to solve the dispersion model equations. Turbulent diffusion is parameterized in SCIPUFF using second-order closure (Donaldson, 1973; Lewellen, 1977).

There are a few advantages to this setup. Lagrangian models avoid the artificial diffusion problems seen in Eulerian models and SCICHEM accurately treats length scales growing from plumes to clouds. The representation as puffs allows for efficient multiscale dispersion: puffs are merged as they grow, and the resolution can be adapted as the puffs move downwind. SCICHEM computational efficiency has further been improved by the implementation of both adaptive time stepping and adaptive output grids (Electric Power Research Institute, 2019a). The efficient puff merging and adaptive resolution decreases the number of puffs needed for each simulation, allowing SCICHEM to run efficiently at high resolutions and and short timescales (Sykes et al., 1998).

Sources can be specified as continuous or instantaneous, or anywhere in between. A continuous source is specified as a constant mass release rate, where the material type and the release location must also be defined. The source geometry is defined using the spread parameter, which allows for different "stack" types. Instantaneous sources use a single puff creation stage and are specified by a release time, a release location, and a file containing material identifiers that correspond to existing SCICHEM material types. This file also provides mass, centroid location, and spread parameters for each puff.

SCICHEM also allows for several different chemical options. It can be run in a tracer mode, where the tracer does not undergo any chemical decay. Alternatively, a linear decay can be applied to represent a simple reduction in concentration (e.g., radioactive half-lives). A reduced chemical mechanism for the near-source chemistry of $NO_2$ can be used for $NO_2$ permitting applications. Full gas and aerosol phase chemistry can also be included, which allows SCICHEM to account for chemical formation and loss of species like $O_3$ and $PM_{2.5}$. However, SCICHEM is not currently capable of modeling the chemistry of a battery fire accident, though the model could be expanded to do so. SCICHEM also cannot explicitly model explosions, limiting its ability to accurately model the source term of a battery fire. However, because detailed source-term information can be input into SCICHEM, a separate model could be used to generate a representative post-explosion source term that could then initialize SCICHEM. For example, as described below in Section 4.1, ALOHA can calculate blast effects from vapor clouds. Thus, as a hypothetical example, the combination of ALOHA and SCICHEM potentially could be used to model battery explosion and fire plume dispersion.

SCICHEM meteorological input is specified as either observational or gridded. SCICHEM can also run using simple observational data (e.g., wind measurements) or more detailed observations of parameters such turbulence or the Pasquill-Guifford-Turner Stability class. When multiple surface and profile observations are available, a diagnostic mass-consistent wind model can calculate the 3-D time-dependent wind fields. Alternatively, three-dimensional gridded wind and temperature fields generated by numerical weather prediction models (or their analyses) can be used as input. The small-scale turbulence in the lower portion of the planetary boundary layer (PBL) can be described using surface heat and momentum

fluxes, but can also be specified with observations of turbulence profiles (using its standard observational meteorological input format).

SCICHEM is a public model (available online at https://github.com/epri-dev/SCICHEM). It can be run on Windows or Linux from the command line and prebuilt binaries for Windows and Linux are available. A developmental GUI is available on Windows and can be used for reviewing a completed project or for plotting the species total concentrations for all projects. A user's guide, technical documentation, and several tutorials are available (Electric Power Research Institute, 2019a, b).

## 3.2 Phast

The Process Hazard Analysis Software (Phast) is a commercial system that can be used to analyze accidental releases from their starting point to distant areas (e.g., Witlox and Holt, 1999; Pandya et al., 2012). The system accounts for several processes that might be useful to the battery dispersion modeling problem, including the simulation of dense gas dispersion, vapor cloud explosions, and toxic effects. It can also model both unpressurized and pressurized pipes as well as account for plume buoyancy and rainout.

The underlying model in Phast is the Unified Dispersion Model (UDM). UDM can simulate two-phase releases that are elevated or surface-based. It is termed "Unified" because it is one model with separate modules to calculate: (1) jet dispersion, (2) dense gas dispersion, (3) passive dispersion, (4) droplet rainout and evaporation, and (5) subsequent pool spreading and re-evaporation back into the plume. It can do this in both the near- and far-fields. Phast also incorporates vapor cloud explosion modeling using the Baker-Strehlow-Tang and Multi-Energy explosion models. Plume buoyancy is accounted for in the thermodynamic modules that calculate average cloud temperature, density, and phase distribution (Witlox and Holt, 1999). Chemical reactions are not incorporated into Phast. Building downwash effects can also be simulated (Witlox, 2010), but downwind obstacles cannot be considered. Terrain effects can be modeled by changing the assumed roughness length and terrain type (land vs. water).

Phast has been extensively validated against field experiments and analytical data. For example, UDM's heavy gas dispersion has shown good agreement with analytical results and wind-tunnel experiments of $CO_2$ dispersion (Witlox and Holt, 1999; Witlox, 2010). It has shown agreement with passive dispersion results from the Prairie Grass experiment, aerosol releases at Desert Tortoise (ammonia), and research on the dispersion of two-phase flashing releases (FLADIS; ammonia) (Witlox and Holt, 1999). It did have difficulty accurately capturing the transition from jet-to-passive dispersion for the Goldfish experiment (two-phase HF release), which degraded its far-field results. However, it performed well closer to the source. It also performed well for two heavy gas dispersion experiments (Witlox and Holt, 1999; Witlox, 2010). Finally, Phast's UDM has undergone rigorous validation for approval as a model in the siting of Liquified Natural Gas (LNG) facilities by the Pipeline and Hazardous Materials Safety Administration (PHMSA) of the US Department of Transportation (DOT) (Wilox et al., 2013).

The Phast modeling system from DNV-GL has several output parameters that may be useful to the battery fire dispersion problem. For example, users can output the concentration at a specified distance, the cloud's footprint at any given time, and several hazard analysis parameters, such as toxic effect (e.g., Pandya et al., 2012). Additionally, users have flexibility in specifying the source term and meteorological conditions. Users can also specify source height, source angle (which affects crosswind entrainment), the vertical wind profile, and many other parameters (Pandya et al., 2012).

Overall, although Phast is not currently explicitly configured to model battery fire dispersion, it is a unified and extensively validated model that calculates many aspects of dispersion that are relevant for this application. However, one drawback is that the modeling system would need to be purchased, unlike some of the other free options (e.g., SCICHEM).

Lastly, because the model is proprietary, the source code is not available. Therefore, users would be limited to modifying the current parameters available in Phast with no capability to add new ones relevant to battery fire dispersion. Furthermore, although the background on Phast indicates that it is suitable for this application, practical firsthand use of the model is needed to determine if it is flexible enough to simulate battery fire dispersion with its current options.

## 3.3 SAFER/TRACE

The Toxic Release Analysis of Chemical Emissions (TRACE) model was developed to evaluate the impacts of toxic chemical spills (Zapert et al.,1991) at both near- and far-field distances. SAFER/TRACE is a proprietary version of TRACE developed and maintained by Systematic Approach for Emergency Response (SAFER) Systems. The modeling system incorporates over 600 different compounds in its chemical library and can model two-phase dense or positively buoyant releases that are surface-based or elevated. The releases can be instantaneous, continuous, or intermittent (Hanna et al., 1991a). SAFER/TRACE uses chemical, environmental, container, and rupture information to calculate release characteristics such as emission rate and temperature. It can also account for fires and explosions. Upon release into the atmosphere, SAFER/TRACE calculates the fraction of the liquid that converts to gas and the final temperature of the cloud. A liquid pool can form if the cloud is transported down to the surface. SAFER/TRACE then accounts for pool spreading and re-evaporation back into the plume (Hanna et al., 1991b).

SAFER/TRACE has been extensively evaluated against several dispersion experiments. For example, Hanna et al. (2008) evaluated the ability of six different models to simulate chlorine dispersion following three railcar accidents. They found that TRACE and Phast were the only two able to adequately model the complex emissions source term, which was the most critical component of the subsequent dispersion agreement among the models. Hanna et al. (1993) evaluated thirteen different models against multiple campaigns consisting of dense gas, passive, and two-phase releases. They found that SAFER/TRACE did slightly worse for a continuous release of a passive gas; however, its performance was comparable to all other models studied for dense gas dispersion.

The SAFER/TRACE modeling suite is built for Windows and has an extensive user interface to allow for facility-dependent simulations. Users can vary the output averaging time, which is necessary to capture the small timescales of processes relevant to battery fire dispersion. Additionally, the system predicts concentrations at user-specified receptor locations. Overall, the model can account for each phase of the battery fire dispersion problem and has been validated against various experimental datasets. However, because SAFER/TRACE is proprietary, the source code would likely not be made available. Additionally, it is unclear if the code is flexible enough to accommodate the battery fire problem. Therefore, additional firsthand use of the model is needed to determine its suitability to simulate battery fire dispersion with its current options.

# 4. Description of Related Modeling Tools Found Unsuitable for this Application

A detailed description is given below for modeling tools that met some of the criteria. For those that were completely unsuitable, only a brief description is given.

## 4.1 CAMEO/ALOHA

CAMEO is a suite of software tools developed by the EPA and NOAA to assist front-line chemical emergency planners and responders in chemical emergencies. It allows them to access, store, and evaluate crucial information for generating emergency plans. CAMEO also supports regulatory compliance through its ability to help users meet chemical inventory reporting requirements. The CAMEO system integrates a chemical database (CAMEO Chemicals), a method to manage the data (CAMEOfm), an air dispersion model (ALOHA), and a mapping capability (MARPLOT).

ALOHA is the dispersion model used in the CAMEO suite for evaluating hazardous chemical releases (Jones et al., 2013). ALOHA ingests user-specific parameters about an event (e.g., toxicological characteristics, atmospheric conditions) to estimate the downwind dispersion of a chemical cloud. ALOHA uses a graphical interface for data entry and display of results. It can estimate and display threat zones for a variety of hazardous scenarios, including toxic gas clouds, flammable gas clouds, and vapor cloud explosions. However, a major limitation of the CAMEO/ALOHA suite is its inability to account for plume rise.

ALOHA is designed to predict hazards regions on the scale of 100 m to 10,000 m for accidental spills, with durations of up to an hour, which fits well with the scale of battery fires. However, another limitation of ALOHA is how it accounts for the effects associated with terrain and buildings. ALOHA uses a wind field that does not vary spatially or temporally and therefore cannot account changes in flow direction due to buildings or terrain.

ALOHA uses a variety of models to estimate the chemical release rate, including modeling puddles, tanks, and gas pipelines. Additionally, it incorporates models to calculate blast effects from vapor clouds and models for thermal radiation and flammable area, which is relevant to the second phase of the battery fire problem. This portion of ALOHA could potentially be beneficial for the battery fire dispersion problem if combined with another model that accounts for plume buoyancy.

CAMEO/ALOHA is a public model. It is available in Mac and Windows formats. ALOHA has example scenarios, technical documentation, and the CAMEO help desk available for user support (Jones et al. 2013).

## 4.2 CALPUFF

CALPUFF is an advanced, non-steady-state meteorological and air quality modeling system developed by scientists now at Exponent, Inc (Earth Tech, Inc., 2000). The modeling system consists of three main components: (1) the meteorological model CALMET, (2) the Lagrangian puff model CALPUFF, and (3) the post-processing program CALPOST.

In addition to these components, there are several other processors that can be used to prepare geophysical and meteorological data to be used in the system. Additionally, CALPUFF interfaces with other commonly-used models such as the Weather Research and Forecasting (WRF) model (Skamarock and Klemp, 2008).

In general, puff models represent a continuous plume as a number of discrete packets of contaminant material. Then, the contribution of a puff to the concentration at a receptor is evaluated using a snapshot approach (Ludwig et al, 1977). A drawback of this approach is the need to release a large number of puffs to adequately represent a continuous plume when close to the source. To alleviate this, CALPUFF allows two alternative sampling schemes to be selected. Both are based on the integrated sampling function in the MESOPUFF II model (Scire et al., 1984a,b) that have been modified for near-field applications. However, a major drawback to CALPUFF is that the smallest averaging time available is one hour. The explosion and other phases of the battery fire dispersion problem occur on much smaller timescales, limiting CALPUFF's usefulness for this application.

## 4.3 AERMOD

AERMOD is a steady-state plume model. It assumes the concentration distribution to be Gaussian in both the horizontal and vertical in the stable boundary layer (SBL). In the convective boundary layer (CBL), the horizontal distribution is also assumed to be Gaussian, but the vertical distribution is described with a bi-Gaussian probability density function, which also was demonstrated by Willis and Deardorff (1981) and Briggs (1993). Additionally, in the CBL, AERMOD accounts for plume lofting, a process where a portion of plume mass that is released from a buoyant source rises to and remains near the top of the boundary layer before becoming vertically mixed throughout the CBL. This process could be useful in the battery fire modeling application. The AERMOD model includes a wide range of options for modeling air quality impacts of pollution sources, making it a popular choice among the air quality modeling community. The AERMOD model is applicable to rural and urban areas, flat and complex terrain, surface and elevated releases, and multiple

sources (including point, area and volume sources). AERMOD and its documentation are publicly available (U.S. Environmental Protection Agency, 2019a, c).

Similar to CALPUFF, a major drawback of AERMOD is that it simulates pollutant concentrations at a minimum averaging time of one hour. For battery fires, where it is critical that the dispersion model be able to simulate concentrations at timescales of minutes or less, this disqualifies AERMOD as a potential candidate. Thus, although it has features useful to this problem, the time resolution of AERMOD is too coarse to accurately model the different phases of a battery fire release and dispersion event.

## 4.4 Brief Summary of Other Models Found Unsuitable

- HPAC/JEM: HPAC is a fast-running modeling system that aids in emergency response to hazardous releases (DTRA, 2001). It is available for use by the Government (typically the Department of Defense [DoD] and Department of Energy) and Government-related or academic organizations. HPAC simulates the effects of HAZMAT releases into the environment and their impact on civilian and military populations. The modeling software simulates hazard areas produced by accidental releases using integrated source terms, high-resolution weather forecasts, and particulate transport. HPAC includes the SCIPUFF model for turbulent transport. JEM is a sister model, based on HPAC and other dispersion models (e.g., D2PUFF) developed within DoD, and there have been efforts to reconcile the two versions of the HPAC model. However, the major limiting factor for HPAC is that it is not available to the general public.

- HYSPLIT: The HYSPLIT model can simulate simple air parcel trajectories, as well as complex transport, dispersion, and deposition simulations (Draxler and Hess, 1998). The transport and dispersion is calculated as a hybrid between the Lagrangian and Eulerian approaches. (The model name, no longer meant as an acronym, originally reflected this hybrid computational approach). The dispersion of a pollutant is calculated by assuming either puff or particle dispersion. HYSPLIT has traditionally been used for mesoscale applications. Recently, it has been applied at finer resolution (100 m) for the Sagebrush Tracer Experiment (Ngan et al., 2018), suggesting that it is applicable at smaller scales. However, because HYSPLIT cannot simulate dense gases, it is not recommended here..

- STILT: The Stochastic Time Inverted Lagrangian Transport (STILT) model grew out of HYSPLIT as an implementation of its Lagrangian particle dispersion model (LPDM) capability (Lin et al., 2003). Most of the STILT functionality has since been merged back into HYSPLIT. However, STILT is a mesoscale model, and not a good fit for this application.

- FLEXPART: The Flexible Particle (FLEXPART) model is a LPDM that simulates both long-range and mesoscale transport, as well as diffusion, dry and wet deposition, and radioactive decay of tracers (Stohl et al. 2005). As a mesoscale model, it is not a good fit for this application.

- WRF-Fire: A wildland fire-behavior module, named WRF-Fire, is integrated into the WRF numerical weather prediction model (Coen et al., 2012). The fire module is implemented at the surface with two-way coupling to the atmospheric model. Near-surface winds from WRF are interpolated to a finer fire grid and are used, in combination with fuel properties and local terrain gradients, to determine a fire's spread rate and direction. This module is geared towards wildfires, as opposed to small-scale battery fires, and is therefore not a good fit for this application.

- WRF-Chem: This is the WRF model coupled with Chemistry (Grell et al., 2005). The model simulates the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the WRF meteorology. The model is used for investigation of regional-scale air quality, field program analysis, and cloud-chemistry interactions. This model computationally expensive and is geared towards regional scale studies, making it less suitable for this application.

- CMAQ: The Community Multiscale Air Quality (CMAQ) modeling system is a three-dimensional Eulerian atmospheric chemistry and transport modeling system that simulates ozone, particulate matter, toxic pollutants, visibility, and acidic and nutrient pollutant species throughout the troposphere (https://www.epa.gov/cmaq; Byun & Schere, 2006). CMAQ can address complex air quality issues across spatial scales ranging from urban to hemispheric. The WRF model is commonly used to drive CMAQ and can also be coupled directly with it in the WRF-CMAQ two-way system. To obtain inputs on emissions, CMAQ relies on an emissions processor to estimate the magnitude, location, and temporal variability of pollution sources. Open-source processors, such as the Sparse Matrix Operator Kernel Emissions (SMOKE) processor, are available for computing emissions inputs to CMAQ from emissions inventories. However, CMAQ is typically used for studies at a spatial scale of 4 km or more, and requires extensive work to prepare the input data, and thus is less appropriate for this application.

- QUIC-Plume LPDM: The Quick Urban & Industrial Complex (QUIC) Dispersion Modeling System is a fast response urban dispersion model. The QUIC system has several components: a 3D wind field model called QUIC-URB, a transport and dispersion model called QUIC-PLUME, a pressure solver called QUIC-PRESSURE, and graphical user interface called QUIC-GUI. It efficiently computes chemical, biological, and radiological (CBR) agent dispersion on building to neighborhood scales, taking only tens of seconds to tens of minutes to run. This is a Department of Energy model and is only available for non-profit research purposes (Nelson and Brown, 2013). Since it is not publicly available, it is not a good fit for this application.

- Offshore and Coastal Dispersion Model: The Offshore and Coastal Dispersion (OCD) model was developed for the Minerals Management Service to determine the effects of offshore and onshore emissions on coastal air quality (DiCristofaro and Hanna, 1991). Devel-

oped in the 1980s and infrequently updated, this model is fairly dated compared to other options and since it specializes in coastal regions, it is not a good fit for this more general application.

- CTDMPLUS: Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations (CTDMPLUS) is a refined point source Gaussian air quality model for use in all stability conditions for complex terrain (Strimatis et al., 1987). Developed in the 1980s, infrequently updated, and specializing in complex terrain, this model is not a good fit for this application.

- Atmospheric Dispersion Modeling System (ADMS-5): An advanced dispersion model that can account for structures, terrain, and gravitational settling of emissions (Cambridge Environmental Research Consultants, 2020). This model was built and designed for running in Europe. Therefore, there might be increased setup time to get ADMS-5 up-and-running (file conversions, domain-specific terrain files, etc.), which must also be taken into consideration. Additionally, the creators of ADMS-5, the Cambridge Environmental Research Consultants Ltd (CERC), do not make the source code available, making it less fitting for this application.

# 5. Recommendations for Future Work

We recommend that future work involve developing a system for modeling battery fires that is based on the publicly available, open-source, and well-documented SCICHEM model. SCICHEM would provide more realistic transport and dispersion and provide the ability to look at larger-scale impacts, including the chemical transformations of some of the released gases as well as impacts from structures and terrain. The Phast and SAFER/TRACE proprietary models also appear to be suitable for the battery fire dispersion problem; however, more information or direct access to the models is needed to fully evaluate them. The inability of CAMEO/ALOHA to model plume rise excludes it as a candidate. However, because ALOHA can calculate the blast effects from vapor clouds, it potentially could be useful for prescribing the source conditions for fires and explosions in SCICHEM. This integration of tools would allow the use of the appropriate model for each phase of the battery fire dispersion problem. However, it would require further testing to ensure the combined approach runs efficiently and accurately.

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