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Dispersion Modeling Systems Relevant to Homeland Security Preparedness and Response





Office of Research and Development CESER/HSMMD/DCB

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by

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Abstract

As one of its core research focuses, the U.S. Environmental Protection Agency's (EPA's) Homeland Security Research Program (HSRP) is interested in refining its tools and methodologies to better characterize the fate and transport of hazardous contaminants during all phases of an emergency response. Atmospheric dispersion modeling is one tool that can be used for effective emergency preparation or response from hazardous chemical, biological, radiological, nuclear, and explosive (CBRNe) releases, especially in urban areas where population densities are high and wind flow becomes altered between buildings and street canyons. The goal of this report is to explain the fundamental concepts of atmospheric transport and dispersion and provide a comprehensive database of dispersion models that can be used for emergency preparation and response to facilitate discussion between public, private, academic, and/or government sectors. The abundance of available modeling options creates confusion and results in challenging decisions regarding the type of model to be used during different scenarios. A comprehensive dispersion model review of this magnitude has also not occurred recently. This report provides a literature review of previous model review efforts to lay the foundation for this updated database, provides introductory concepts on boundary layer meteorology and the types of dispersion models available (e.g. Gaussian Plume or Puff, Lagrangian, or CFD models), and outlines a comprehensive list of 96 dispersion models that could be considered for wide-area release risks. Sixteen of those models were selected for a more detailed two-page review due to their potential applicability and usefulness for emergency response. This model review is not meant to recommend or endorse a specific model, but to provide users with a resource of available modeling options. Even though no single model tends to have all the capabilities that are beneficial during the consequence management of a wide area release, this report is meant to identify the strengths and limitations so users can make informed decisions.

This report covers a research period from September 2018 to June 2020 and work was completed as of July 2020 as part of the author's Ph.D. dissertation.

Foreword

The U.S. Environmental Protection Agency (EPA) is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet this mandate, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The Center for Environmental Solutions and Emergency Response (CESER) within the Office of Research and Development (ORD) conducts applied, stakeholder-driven research and provides responsive technical support to help solve the Nation's environmental challenges. The Center's research focuses on innovative approaches to address environmental challenges associated with the built environment. We develop technologies and decision-support tools to help safeguard public water systems and groundwater, guide sustainable materials management, remediate sites from traditional contamination sources and emerging environmental stressors, and address potential threats from terrorism and natural disasters. CESER collaborates with both public and private sector partners to foster technologies that improve the effectiveness and reduce the cost of compliance, while anticipating emerging problems. We provide technical support to EPA regions and programs, states, tribal nations, and federal partners, and serve as the interagency liaison for EPA in homeland security research and technology. The Center is a leader in providing scientific solutions to protect human health and the environment.

Gregory Sayles, Director

Center for Environmental Solutions and Emergency Response

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Acronyms and Abbreviations

2D	Two-Dimensional
3D	Three-Dimensional
ABC	Atomic, Biological, and Chemical
ADAM	Air Force Dispersion Assessment Model; Accident Damage Analysis Module
ADAPT	Atmospheric Data Assimilation and Parameterization Tool
ADEME	French Ministry and Environmental Agency
ADMLC	Atmospheric Dispersion Modeling Liaison Committee
ADMS	Atmospheric Dispersion (and Dose Assessment) Modeling System
AER	Atmospheric and Environmental Research
AERMIC	American Meteorological Society/EPA Regulatory Model Improvement
	Committee
AERMOD	American Meteorological Society/Environmental Protection Agency
	Regulatory Model
AES	Atmospheric Environment Service
AFTOX	Air Force Toxics Model
AIR	Atmosphere, Impact, and Risk
AMS	American Meteorological Society
ANL	Argonne National Laboratory
APGEMS	Air Pollutant Graphical Environmental Monitoring System
AQPAC	Air Quality Package
ARA	Applied Research Associates
ARAC	Atmospheric Release Advisory Capability
ARCHIE	Automated Resource for Chemical Hazard Incident Evaluation
ARCON	Atmospheric Relative Concentrations
ARGOS	Accident Reporting and Guidance System
ARL	Air Resources Laboratory
ASPEN	Assessment System for Population Exposure Nationwide
ATD	Atmospheric Transport and Diffusion
BAR	BioWatch Actionable Result
BERT	BioWatch Event Reconstruction Tool
BLP	Buoyant Line and Point (Source Model)
BNL	Brookhaven National Laboratory
BNLGPM	Brookhaven National Laboratory Gaussian Plume Model
CAA	Clean Air Act
CALINE	California Line (Source Dispersion Model)
CALPUFF	California Puff (Model)
CAMEO/ALOHA	Computer-Aided Management of Emergency Operations/Areal Locations of
	Hazardous Atmospheres
CAPARS	Computer-Assisted Protective Action Recommendations System
CASRAM	Chemical Accident Stochastic Risk Assessment Model
CATS-JACE	Consequence Assessment Tool Set/Joint Assessment of Catastrophic Events

CBRNe	Chemical, Biological, Radiological, Nuclear, and Explosive
CERC	Cambridge Environmental Research Consultants
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CESER	Center for Environmental Solutions and Emergency Response
CFATS	Chemical Facility Antiterrorism Standards
CFD	Computational Fluid Dynamics
CISRO	Commonwealth Scientific and Industrial Research Organisation
CMAQ	Community Multiscale Air Quality (Modeling System)
CMI	Christian Michelsen Institute
CML	Convective Mixed Layer
CO	Carbon Monoxide
COOP	Continuity of Operations Plan
CSA	Combat Support Agency
CsCl	Cesium Chloride
CTDMPLUS	Complex Terrain Dispersion Model Plus (Algorithms for Unstable Situations)
CUDM	Canadian Urban Dispersion Model
DCB	Disaster Characterization Branch
DEGADIS	Dense Gas Dispersion (Model)
DELFIC/FPTool	Defense Land Fallout Interpretive Code/ Fallout Planning Tool
DERMA	Danish Emergency Response Model of the Atmosphere
DHHS	U.S. Department of Health and Human Services
DHS	U.S. Department of Homeland Security
DNS	Direct Numerical Simulation
DOC	U.S. Department of Commerce
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
DRIFT	Dispersion of Releases Involving Flammables or Toxics
DSTL	Defence Science and Technology Laboratory
DTRA	Defense Threat Reduction Agency
EC	European Commission
EMS	Emergency Medical Service
EOC	Emergency Operations Center
EPA	U.S. Environmental Protection Agency
EPCRA	Emergency Planning and Community Right-to-Know Act
EPICode	Emergency Prediction Information Code
EPRI	Electric Power Research Institute
ERG	Environmental Response Guidebook
ERT	Environmental Response Team; Environmental Research and Technology, Inc.
ESCAPE	Expert System for Consequence Analysis and Preparing for Emergencies
EU	European Union
EULAG	EUlerian LAGrangian (Model)
FEM3MP	Finite Element Model in 3-Dimensions and Massively Parallelized

FEMA	Federal Emergency Management Agency
FLACS	FLame ACceleration Simulator
FLEXPART	Flexible Particle (Dispersion Model)
FOI	Swedish Defence Research Agency
FRERP	Federal Radiological Emergency Response Plan
FRMAC	Federal Radiological Monitoring and Assessment Center
FRP	Federal Response Plan
GAO	Government Accountability Office
GENII	Generalized Environmental Radiation Dosimetry Software System - Hanford
	Dosimetry System (Gen. II)
GIS	Geographic Information System
GMU	George Mason University
GUI	Graphical User Interface
HASP	Hazard Assessment Simulation and Prediction
HIGRAD/	High-Resolution Model for Strong Gradient Applications Fire Behavior
FIRETEC	(Model)
HOTMAC	Higher Order Turbulence Model for Atmospheric Circulation
HPAC	Hazard Prediction and Assessment Capability
HSE	Health and Safety Executive
HSIN	Homeland Security Information Network
HSMMD	Homeland Security and Materials Management Division
HSPD	Homeland Security Presidential Directive
HSRP	Homeland Security Research Program
HYROAD	Hybrid Roadway (Intersection Model)
HYSPLIT	Hybrid Single-Particle Lagrangian Integrated Trajectory
IBL	Internal Boundary Layer
ICS	Incident Command System
IED	Improvised Explosive Device
IEM	Innovative Emergency Management, Inc
IMAAC	Interagency Modeling and Atmospheric Assessment Center
INL	Idaho National Laboratory
INPUFF	(Gaussian) Integrated Puff (Model)
ISC	Industrial Source Complex (Model)
JEM	Joint Effects Model
JOULES	Joint Outdoor-indoor Urban Large-Eddy Simulation
JRC	Joint Research Centre
JRII	Jack Rabbit II
KBERT	Knowledge-Based-system for Estimating hazards of Radioactive material
	release Transients
KDFOC	"K" Division (Defense Nuclear) Fallout Code
LANL	Los Alamos National Laboratory
LAPMOD	LAgrangian Particle MODel
LBNL	Lawrence Berkeley National Laboratory

LES	Large Eddy Simulation
LFA	Lead Federal Agency
LLNL	Lawrence Livermore National Laboratory
LODI	Lagrangian Operational Dispersion Integrator
LPDM	Lagrangian Particle Dispersion Model
MACCS	MELCOR Accident Consequence Code System
MAHB	Major Accident Hazards Bureau
MATHEW/	Mass-Adjusted Three-Dimensional Wind Field/Atmospheric Diffusion Particle-
ADPIC	in-Cell
MIDAS-AT	Meteorological Information Dispersion and Assessment System Anti-Terrorism
MOU	Memorandum of Understanding
MSS	Micro-Swift Spray
NAAQS	National Ambient Air Quality Standards
NAM	North American Model
NAME	Numerical Atmospheric-Dispersion Modeling Environment
NARAC	National Atmospheric Release Advisory Center
NBC	Nuclear, Biological, and Chemical
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction
NCHRP	National Cooperative Highway Research Program
NEF	National Essential Function
NHSRC	National Homeland Security Research Center
NOAA	National Oceanic and Atmospheric Administration
NO _x	Nitrogen Oxides
NRC	Nuclear Regulatory Commission
NRF	National Response Framework
NWP	Numerical Weather Prediction
NWS	National Weather Service
O 3	Ozone
OBODM	Open Burn/Open Detonation Dispersion Model
OCD	Offshore and Coastal Dispersion (Model)
OECD	Organisation for Economic Co-operation and Development
OFCM	Office of the Federal Coordinator for Meteorology
OMEGA	Operational Multiscale Environment (Model) with Grid Adaptivity
ORD	Office of Research and Development
ORNL	Oak Ridge National Laboratory
OSC	On Scene Coordinator
OSHA	Occupational Safety and Health Administration
OSPM	Operational Street Pollution Model
PANACHE	Atmosphere Pollution and Industrial Risk Analysis
PBL	Planetary Boundary Layer
PHAST	Process Hazard Analysis Software
PI	Principal Investigator

PLUVUE	Plume Visibility (Model)
PM	Particulate Matter
PMEF	Primary Mission Essential Function
PNNL	Pacific Northwest National Laboratory
PPE	Personal Protective Equipment
PUMA	Puff Model of Atmospheric Dispersion
QUIC	Quick Urban Industrial Complex
RA/HA	Risk Assessment/Hazard Assessment
RANS	Reynolds-averaged Navier-Stokes
RAPTAD	Random Puff Transport and Diffusion
RASCAL	Radiological Assessment System for Consequence Analysis
RCRA	Resource Conservation and Recovery Act
RDD	Radiological Dispersal Device
RIMPUFF	Risø Mesoscale Puff Model
RL	Residual Layer
RLINE	Research Line-source (Dispersion Model)
RMP	Risk Management Plan
RSAC	Radiological Safety Analysis Computer (Program)
RTDM	Rough Terrain Dispersion Model
RTVSM	Real-time Volume Source Model
SAIC	Science Applications International Corporation
SBL	Stable Boundary Layer
SCIPUFF	Second-order Closure Integrated Puff (Model)
SCRAM	Support Center for Regulatory and Atmospheric Modeling
SDM	Shoreline Dispersion Model
SHARC/ERAD	Specialized Hazard Assessment Response Capability/ Explosive Release
	Atmospheric Dispersion
SIP	State Implementation Plan
SL	Surface Layer
SNL	Sandia National Laboratory
SOARCA	State-of-the-Art Reactor Consequence Analyses
SRC	Sigma Research Corporation
SRS	Savannah River Site
STILT	Stochastic Time-Inverted Lagrangian Transport (Model)
TAPM	The Air Pollution Model
TIC	Toxic Industrial Chemical
TKE	Turbulent Kinetic Energy
TOPOFF	(National) Top Officials (Exercise)
TRAC	Terrain Responsive Atmospheric Code
TRACE	Toxic Release Analysis of Chemical Emissions
U.S.	United States
UBL	Urban Boundary Layer
UDM	Urban Dispersion Model

UHI	Urban Heat Island
UK	United Kingdom
UoR-SNM	University of Reading Street Network Model
USDA	U.S. Department of Agriculture
USGS	U.S. Geological Survey
VAFTAD	Volcanic Ash Forecast Transport and Dispersion
VAPO	Vulnerability Analysis and Protection Option
VLSTRACK	Vapor, Liquid, and Solid Tracking
WADOCT	Wind and Diffusion Over Complex Terrain
WINDS	Weather Information and Display System
WMD	Weapon of Mass Destruction
WRF	Weather Research and Forecasting Model
YSA	Yamada Science and Art (Corporation)

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1.0 Introduction

After the events of September 11, 2001, the United States quickly became aware of its vulnerability to external terrorism-related threats. To minimize and prepare for potentially adverse future situations, the Federal government established the U.S. Department of Homeland Security (DHS). The agency's goal was to prepare and protect the country against terrorism, instill a presence of border security, and prepare for and manage disaster scenarios. Although the responsibilities of DHS are broad, an important component of its homeland security efforts is the preparation, detection, response, and mitigation of hazardous substance releases into the ambient atmosphere, as these situations have the potential to affect the health and welfare of the American people.

To help fulfill the core objectives, DHS works alongside various government entities, including the United States (US) Environmental Protection Agency (EPA). In September 2002, the US EPA formed the National Homeland Security Research Center (NHSRC) to lead scientific-based research and provide technical expertise for a variety of environmental and human health-related homeland security threats. In 2019, EPA's Office of Research and Development (ORD) reorganized and much of the same research is now handled the Homeland Security Research Program (HSRP). EPA's HSRP and its partners work to develop risk-prevention strategies that strengthen the country's ability to withstand and recover from future disasters and wide-area incidents, whether the hazards stem from natural, accidental, or terroristrelated sources. These wide-area events could span the spatial distance of several city blocks or more, such as within an urban area like lower Manhattan, or throughout a municipality's drinking water distribution system (EPA 2020). Situations that involve the release, or potential release, of hazardous chemicals, microbial pathogens, or radiological materials further complicate disaster scenarios and require specialized expertise during the response and recovery process. As one of its core research focuses, HSRP is particularly interested in refining its tools and methodologies for a better understanding of the fate and transport of hazardous wide-area contaminants (EPA 2020). This need for tool and methodology refinement extends to all phases of an emergency response, from the near-term to the extended remediation and recovery stages.

Upon its creation, DHS was slated to develop new countermeasures for chemical, biological, radiological, nuclear, and explosive (CBRNe) releases, which would include improved knowledge of atmospheric transport and diffusion (ATD) through computer dispersion modeling. A dispersion model is a mathematical representation of the transport of air pollutants in the ambient atmosphere which is used to calculate concentrations at various locations away from the emission source(s) (Holmes and Morawska 2006). The equations governing pollutant dispersion are frequently based on a Gaussian (bell-shaped) downwind concentration distributions and are solved through computer modeling software. Understanding complex atmospheric flow and dispersion processes, especially in urban areas, is important when modeling hazardous air quality scenarios. These efforts are supported by the U.S. Department of Commerce (DOC) Office of the Federal Coordinator for Meteorology (OFCM) and several collaborating federal agencies that developed guidance for dispersion modeling implementation (OFCM 2002).

In the federal government, operational dispersion modeling is a multiagency approach. Hazardous accidental release scenarios may arise from accidental industrial and transportation-related contaminant spills and intentional acts of terrorism. To provide a single point for the coordination and dissemination of hazard prediction products, DHS established a multiagency working group in 2004 called the Interagency Modeling and Atmospheric Assessment Center (IMAAC). IMAAC was not intended to replace individual dispersion modeling efforts but is able to be activated quickly if a hazardous release occurs and an emergency plume estimation is required under tight time constraints. Dispersion modeling in its research, regulatory, or academic role, is a multifaceted scientific tool used, developed, and improved by many private, university, state, and federal government entities, including the EPA.

While considerable research and development effort has been leveraged in dispersion modeling improvements over the past several decades, especially for CBRNe releases, there is still room for further development. The critical need for advancements in atmospheric modeling and plume prediction has been rekindled from the events on September 11, as well as other numerous hazardous situations, including the threat of wide-area *Bacillus anthracis* (anthrax) releases (Amerithrax), the 2011 Fukushima nuclear reactor accident, the 2017 Portland, Oregon asbestos fire, or more recently the 2020 Visakhapatnam styrene gas leak, which could have had a result similar to the 1984 Bhopal disaster. These scenarios are just a few cases demonstrating the critical need for dispersion models to be continuously tested, developed, and improved, usually by evaluating their performance against extensive field and laboratory data. Since it is impossible to predict the timing and location of the next catastrophic incident, emergency responders must be prepared for a multitude of hazardous releases. Dispersion modeling offers a critical insight in emergency preparation or planning so responders can become better equipped for various release scenarios. It is also a critical component or tool for efficient and precise emergency response (Leitl et al. 2016), especially for determining the extent of a toxic plume and informing where to evacuate, sample, decontaminate surfaces, and manage waste.

Building on the fundamental concepts and physical understanding of atmospheric transport and diffusion that emerged in the early-to-mid twentieth century when the foundation of ATD research was laid (Richardson 1922; Taylor 1921; Pasquill 1961, and others), today's model development activities focus on more complex circumstances. These situations are particularly challenging in urban areas with high population densities and the potential for acute exposure effects (Schmidtgoessling 2009). The complex nature of a cityscape results in substantial challenges in determining pollution dispersion throughout the urban canopy (Garbero 2008). Wind flow patterns become altered by the urban geometry, and turbulent flows are generated between buildings and streets (Belcher et al. 2013; Barlow and Coceal 2009; Britter and Hanna 2003). The urban canopy also tends to modify the local boundary layer by reducing wind speeds, increasing turbulent intensities and turbulent kinetic energy (TKE) in the lee of buildings, and increasing episodes of neutral stability instead of extreme stability through added turbulence and heat fluxes (Arya 2001; Briggs 1973). The simplifying assumptions in many dispersion models make urban, industrial, and small-scale modeling quick and efficient for rapid results but also introduce errors that could propagate to poor model performance (Chang et al. 2005). An acceptable balance between speed, model performance, ease of use, and purpose of application must be established when employing a dispersion model for emergency response. As a result, the use, analysis, and implementation of atmospheric dispersion models, along with improvements and more in-depth understanding of micro- and mesoscale transport processes, are key research priorities within the EPA. Improved dispersion research can also aid the EPA's emergency response mission in preparing for and responding to large-scale CBRNe incidents as part of the Homeland Security Research Program (HSRP) (EPA 2020).

This document first outlines the project background, justification, and goals in **Section 2.0**, along with a short literature review of previous dispersion model compilations. **Section 3.0** identifies the role of dispersion modeling in emergency preparation and response, details the available operational dispersion modeling resources, and defines EPA's role in emergency response. **Section 4.0** provides an overview of atmospheric turbulence and the fundamentals of dispersion within the Planetary Boundary Layer (PBL) and urban areas. The types and corresponding strengths and limitations for different dispersion models are covered in **Section 5.0**. **Section 6.0** describes the model review process, specific details included in the review, and the criteria used to determine inclusion or omission of the model in the detailed review. An extensive quick reference table for 96 different dispersion models is provided in **Section 7.0**, and 16 of those models are selected for additional review in **Section 8.0** due to their applicability and usefulness for emergency response.

2.0 Project Background and Goals

Dispersion model users often must make challenging decisions on the type of model to select for their unique scenario depending on release type, terrain, urban geometry, and time considerations. The abundance of publicly available, proprietary, or no-longer-supported atmospheric dispersion models (or simply "dispersion models") often creates considerable confusion for investigators attempting to select and use a model for their purpose, especially as research and scientific knowledge of atmospheric dispersion continues to advance. Although the assessment is now somewhat dated, the OFCM noted that there were over 140 types of public and proprietary dispersion models developed for a variety of purposes (OFCM 2002). However, only a small subset of those models is readily accessible or still being used in regulatory efforts and urban emergency planning initiatives while others are not designed for emergency planning or response.

2.1 Project Motivation

The purpose of this report is to provide a comprehensive database of dispersion models while also briefly explaining the fundamental concepts of atmospheric transport and dispersion incorporated in each model. This document outlines and alphabetically sorts dispersion modeling systems and acts as a comprehensive guide for modelers to rapidly relay risk, sampling, and various model choices to decision makers. The ATD background information (Section 4.0) and model type summaries (Section 5.0) are intended to provide a quick reference for those new to air dispersion modeling or for those seeking to expand their knowledge base but is not meant to replace primary literature sources such as textbooks. Literature is introduced from various academic journal articles, textbooks, government documents, and various reports to provide a diverse synthesis of information. Currently available dispersion models, situations where they are most applicable, model availability and runtime, and notable studies and publications from academic articles are also detailed. Many models can simulate atmospheric transport and diffusion; however, this report emphasizes dispersion models that have specific emergency preparation and response applications, urban or complex environment capabilities, and those that can simulate scenarios related to a variety of hazardous CBRNe cases. Because individual models are necessarily limited in scope and may not have all the components required to be beneficial during consequence management of a wide area response (Mikelonis et al., 2018), this report aims to document the capabilities of dispersion models within the framework of emergency response and preparedness.

The goal is to provide EPA researchers, emergency response planners (federal, regional, and/or local), and policymakers an additional resource to make informed decisions regarding dispersion model use. Emergency planners may find this document a useful reference and ideal starting point when learning about potential modeling resources. This document may also be beneficial when attempting to select a dispersion model to assess local emergency planning exercises such as within areas with high levels of potential human exposure. EPA scientists may use this document as a resource when developing research projects or field studies that involve an airborne release. This report is also intended to facilitate discussion between public, private, academic, and/or government sectors to aid in the selection of a useful dispersion model during the preparation, response, or recovery phases.

The need to periodically review the state of dispersion modeling arises from the continuous growth in our understanding of boundary layer turbulence, dispersion, ongoing model development, and the sheer number of dispersion model variations. Some of these models have not been updated recently and are retired, while others are proprietary and may be used only by their developers or paid subscribers. Other dispersion models are only suitable for specific releases (i.e., radiological release, explosions, dense gas). In a charge recommended by the Atmospheric Dispersion Modeling Liaison Committee (ADMLC) appointed in the United Kingdom, "a qualitative assessment of the 'use-ability' of a model should be undertaken, considering the extent to which the model is user-friendly, the data requirements of the model, and accessibility and availability of such models" (ADMLC 2013). A similar request was raised in the U.S. at the 22nd Annual George Mason University (GMU) Conference of Atmospheric Transport and Dispersion Modeling in June 2018. The OFCM called upon a joint action working group of various agencies to revise the 2002 and 2004 atmospheric modeling guidebooks for homeland security applications (see: OFCM 2002; 2004), but the status of this update is not known. As these documents are 16-18 years old (at the time of this report), a considerable number of changes may be warranted. Additionally, OFCM used to publish a directory of consequence assessment dispersion models, but that document has not been updated in over two decades (OFCM 1999).

The U.S. Government Accountability Office (GAO) also noted in a 2008 report for DHS that confusion and lack of coordination between government agencies has existed when these agencies respond to simulated homeland security incidents, demonstrating that the federal government struggles to efficiently "coordinate and properly use atmospheric transport and dispersion models" (US GAO 2008). From discussions with on-scene coordinators and EPA researchers, as well as literature and guidance documents, considerable confusion still exists regarding the options for current dispersion models, their capabilities, and applicability of use. The need for a coordinated and centralized response has led to the establishment of IMAAC and the National Atmospheric Release Advisory Center (NARAC). A resource such as this report may be useful for individuals who want to select a dispersion model for research or planning scenarios.

2.2 Background and Previous Model Review Efforts

The OFCM, which leads a collaboration with at least 14 federal agencies including the National Oceanic and Atmospheric Administration (NOAA), U.S. Department of Defense (DOD), and U.S. Department of Energy (DOE), and EPA developed a series of comprehensive dispersion modeling directories (OFCM 1993, 1999, 2002, 2004). Those reviews, last published in the late 1990s, provided an in-depth compilation and description of atmospheric dispersion models available to those with consequence assessment requirements, especially those requiring real-time information on chemical, radiological, or biological weapon emergencies. The first version of the report published by OFCM in 1993 was titled "*Directory of Atmospheric Transport and Diffusion Models, Equipment, and Projects*" (FCM-I3-1993) (OFCM 1993), followed by an update in 1995. The last and final version broadened the consequence assessment scope of the model directory to incorporate fires and explosions (OFCM 1999). The OFCM then issued a report after the 9/11 tragedy noting that while there were currently over 140 dispersion modeling systems used for regulatory, research, and emergency response, only approximately 29 non-proprietary models were used by first responders, with even fewer used operationally in quick-response modeling facilities (OFCM 2002). The report featured these models sorted by scenario to address end users' needs.

The U.S. DOE Emergency Management Advisory Committee and Subcommittee on Consequence Assessment and Protective Actions also published an early report logging 93 dispersion models known to be used within the DOE consequence assessment community (Mazzola et al. 1995¹). Many of the models on the survey list are not used frequently or are specific to individual DOE sites. In addition, another review of existing dispersion modeling software concluded that no one system had all the features that were deemed critical for emergency preparation and response (National Research Council 2003). Some of the models fell short on the confidence in predicted dosages and urban and complex topography. The

¹ The document entitled "Atmospheric Dispersion Modeling Resources" can be accessed online at: <u>http://www6.uniovi.es/gma/admr.pdf</u>

report suggested that users focus on models with short run times for response applications and more accurate but slower models for preparedness and recovery phases.

Vardoulakis et al. (2003) compiled a comprehensive review paper of urban dispersion models capable of use in street canyons following gaseous releases. The focus was to document the effects of buildings within the urban street canyon and then to provide information on the 47 dispersion models found to simulate some form of gaseous release within the urban canyon, particularly for traffic-related emissions. Holmes and Morawska (2006) produced the first overview of dispersion models capable of characterizing particle dispersion. The authors reviewed 18 commercial and publicly available box, Gaussian, and Lagrangian/Eulerian dispersion models, as well as 11 aerosol dynamics models or modules, noting that substantial differences existed between the models, and that considerable thought must be given when selecting a model for each application. It was not possible to rank the models based on performance or usefulness due to large model differences and the lack of particle evaluation field studies to test the integrity of each model (Holmes and Morawska 2006).

The ADMLC working group called upon its membership of government departments, utilities, and research organizations to develop a review of urban dispersion modeling efforts, current advances, and future needs, including a section detailing currently available models and a review of dispersion modeling advances from accidental releases in urban areas since the previous review in 2002 (ADMLC 2013). A follow-on publication by Belcher et al. (2013) addressed this request, but the document does not generally describe more than ten modeling systems or provide a useful and comprehensive table as seen in other resources.

Most recently and within the homeland security realm, Van Leuken et al. (2016) conducted a review of dispersion modeling studies that assessed pathogenic bioaerosols to humans and livestock. The authors identified 16 models capable of simulating bioaerosol dispersion, provided background information on dispersion modeling and potential bioaerosols, and developed a comprehensive table of atmospheric pathogen dispersion studies, including the models employed. Most emergency preparedness models only considered *B. anthracis* as their bioagent of focus, and all studies lacked full quantitative risk assessments (most were simply qualitative). Hertwig et al. (2018) evaluated eight variations of atmospheric dispersion models (including Gaussian, Lagrangian, large eddy simulations (LES), and street network models) in mock urban areas with building obstacles. The goal was to compare results based on the necessary balance of model speed and accuracy during emergency scenarios. The authors suggested that the emerging, simple variations of street network models may provide accurate results comparable to complex Lagrangian models (Hertwig et al. 2018), but the emerging models are not relatively well known or extensively tested.

2.3 Project Goals

The objectives of this report are as follows:

- 1. Introduce CBRNe terminology and illustrate how atmospheric dispersion models can simulate these releases (**Section 3.2**).
- 2. Define the responsibilities of government agencies and IMAAC during a hazardous atmospheric release (**Section 3.4-3.5**).
- 3. Document EPA's contribution to dispersion modeling, including its history, preferred and recommended models, role in emergency response operations and modeling efforts (Section 3.6).
- 4. Provide a brief background on PBL processes that control the dispersion of hazardous releases, including an overview of urban flow phenomenology from city structures (Section 4.0).

- 5. Introduce and discuss the advantages and disadvantages of current dispersion models including Gaussian Plume and Puff models, Eulerian grid models, Lagrangian stochastic models, and computational fluid dynamic (CFD) models (**Section 5.1-5.7**).
- 6. Briefly identify dispersion model uncertainties and potential sources of error (Section 5.8).
- 7. From peer-reviewed literature, technical reports, and developer websites, identify dispersion models used by private companies, universities, and federal, state, and local agencies that are designed for CBRNe applications. Summarize the models that are primarily used and developed within the U.S. into a concise reference table (Section 7.0).
- 8. Develop a quick reference guide (less than three pages each) for a selection of models that are recommended for use in emergency preparation or response scenarios by expanding upon the model's specifications, usefulness, and applicability to CBRNe releases (**Section 8.0**).

2.4 Literature Quality Assurance

EPA quality assurance policies and procedures were followed for this research effort. Any literature obtained and cited within this report has been subject to a rigorous selection process. As also outlined in the dispersion model selection process (**Section 6.1**), the sources of secondary data and any cited literature in the report included peer reviewed journal articles, federal agency reports, technical documents, model manuals, and published books (including textbooks). The topics pertained to dispersion modeling systems and well-documented micrometeorological concepts. Additional information was gathered through reputable websites associated with the models' developers. Due to the complexity and lengthy history of dispersion model use, previous model applications and well-established concepts were introduced, but emphasis was placed on recent publications, documents, and website information. Older peer-reviewed journal articles referenced in more recent articles were also considered if deemed to contain relevant background information for introducing the material. Some dispersion models that were documented previously in other resources that currently could not be found with a relatively in-depth internet search were not included in the model review and reference table (**Section 8.0**).

During the literature search, secondary data sources were qualitatively assessed according to the source document type. Knowledge of the document type provided an indication of trustworthiness of the information and secondary data contained therein, based on general professional judgment of each document type. Each source of information and/or secondary data was also considered according to the following categories: focus, verity, integrity, rigor, utility, clarity, soundness, uncertainty and variability, and evaluation and review. Additionally, the literature search was limited to articles, websites, and documents published in the English language. An emphasis was placed on models developed or used within the U.S., although some well-known and flexible international models were featured.

Internet search criteria included lists of strategic keywords anticipated to elicit identification of relevant secondary data and information, and the arrangement of the keywords with Boolean operators were used to execute the searches. Boolean searches were performed using strategically selected keywords with the operators AND and OR. After each search, the resulting identified literature was reviewed to determine the effectiveness of the search and the relevancy of the results. Based on the search run results, the Boolean search strategy was revised, and another run was performed. Internet searches were also run using parentheses ("") to ensure certain keywords were obtained.

3.0 Emergency Response and Dispersion Modeling

3.1 Dispersion Modeling Definition

In the simplest terms, a dispersion model is a mathematical representation of the transport and diffusion of air pollutants in the ambient atmosphere that is used to calculate effluent concentrations at various locations away from a source (Holmes and Morawska 2006; Turner 1979). Equations governing the dispersion of pollutants, frequently based on a Gaussian downwind concentration distribution, can be calculated manually or through a variety of computer algorithms. Computing programs and software permit thousands (or millions) of calculations in a short period of time, resulting in rapid estimates of downwind concentrations that can inform policymakers, regulatory entities, researchers, or emergency responders following the release or potential release of a hazardous substance. Most dispersion models have limitations related to their simplified meteorology, terrain, and release assumptions, basic physics, and parameterizations (mathematical simplification) of complex processes (Arya 1999). These assumptions can propagate errors in the dispersion calculation, but the errors are oftentimes outweighed when considering the computational speed and relative accuracy of their prediction.

This section introduces CBRNe terminology, describes the stages of an emergency response, and identifies the available federal resources for emergency dispersion modeling, including IMAAC. The section also clarifies EPA's responsibilities in prevention and mitigation, as well as roles during an emergency response scenario. EPA is not technically a first-responding agency and generally does not mobilize to a scene until 72 hours after the event, once state and local partners have addressed immediate lifesaving operations. An emphasis is placed on EPA's role in hazardous release mitigation strategies and risk evaluation, as well as the recommended models developed by the agency. This section satisfies objectives 1 through 3 as described in **Section 2.3**.

3.2 CBRNe Terminology

Dispersion modeling provides significant insight to understand the fate and transport of CBRNe (pronounced "see-burn-e", or simply CBRN or CBR) releases, as these situations pose significant environmental and human exposure risks (Schmidtgoessling 2009). CBRNe's (chemical, biological, radiological, nuclear, and explosive's) modern etymology is adapted from the Cold War acronyms ABC (Atomic, Biological, Chemical) and NBC (Nuclear, Biological, Chemical), which were used to describe agents intentionally (or accidentally) released that inflict harm (Hendricks and Hall 2007a). These agents are sometimes referred to as weapons of mass destruction (WMDs), but warfighting, emergency response, and scientific professionals use the CBRN or CBRNe identification to better characterize the release agents. CBRNe releases are often associated with terrorist-related events intended to inflict mass casualties and/or cause major infrastructural and systematic disruptions. However, most CBRNe releases are inadvertent and typically the result of poor maintenance or structural upkeep, vehicular accidents, or human error. Oftentimes, hazardous substances such as toxic industrial chemicals (TICs) are transported near or through cities and stored close to inhabited locations (Brown 2014), where they have the potential to enter the environment accidentally or intentionally. The following subsections define terminology used to describe a broad overview of CBRNe releases to set the stage for their application within dispersion models.

3.2.1 Chemical

Gaseous chemical releases may refer to various types of chemical weapons or TICs such as nerve, choking, and blister agents that can incapacitate an individual. Certain pesticides, mustard gas, sarin, and

chlorine are examples of chemical agents. In high concentrations, these chemicals can kill or directly harm their target. The release of sarin gas (extremely toxic at low concentrations) in Nazi Germany was an instance of an intentional chemical release. The 1984 Bhopal disaster in India is often considered one of the world's worst unintentional industrial chemical-related disasters. Over a half million people were exposed to deadly concentrations of methyl isocyanate gas used in the production of carbamate pesticides. The incident led to almost 4,000 immediate deaths with several thousands more dying from complications (Broughton 2005).

3.2.2 Biological

The intention of biological warfare is to release pathogens such as bacteria, viruses, or toxins so that a person contracting the agent will have adverse health effects. This release can be achieved through the poisoning of fomites (an inanimate object such as clothing or utensils) or food or water supplies with infectious materials (Hendricks and Hall 2007b). One of the best-known intentional biological threats was the release of weaponized particles of *Bacillus anthracis* (anthrax) spores in the United States mail stream in 2001, commonly referred to as Amerithrax. The *Yersinia pestis* bacteria or Black Death during the 1300s, which killed over a third of the European population, can be considered an example of an unintentional biological event (Perry and Fetherston 1997). The pandemic was spread by fleas carried by rodents that resided among the population. The current COVID-19 pandemic may also fit this realm, as well.

3.2.3 Radiological

A radiological release combines radioactive material with explosives but without the detonation of a nuclear device. This type of release is generally achieved in the form of improvised explosives containing radioactive materials such as a dirty bomb, also known as a radiological dispersal device (RDD) containing an agent like ¹³⁷Cs and ¹³⁷cesium chloride (¹³⁷CsCl). The objective of an RDD is not necessarily to inflict mass casualties, but to cause widespread structural and systematic disruption that is costly to repair and decontaminate, often akin to a "weapon of mass *disruption*" (USNRC 2018). The blast or initial release is likely to cause more psychological than physical harm, as levels of radiation from the RDD are not likely to be high enough to cause illness or death, especially far from the blast zone. Most of these events, such as the foiled attempts of Chechen terrorists who tried to explode an improvised ¹³⁷Cs RDD in a park in Moscow in 1995 are intentional (Stewart 2014). An RDD has not been successfully detonated by a militant group thus far. Accidental radiological spills may occur at laboratories and hospitals that use radioactive chemicals, especially during radiation therapy, but are not expected to precipitate wide-area incidents.

3.2.4 Nuclear

Nuclear releases involve accidents at nuclear power plants, the detonation of a nuclear device, or a weapon caused by an explosion due to nuclear fission, where atoms undergo unstoppable division. A nuclear weapon releases an incredible amount of energy over a short period of time, immediately killing individuals close to the blast site and sickening others through radiation poisoning. Although many intentional tests have been carried out, a nuclear device has only been detonated twice as a WMD, i.e., the U.S.-led World War II bombs dropped on Hiroshima and Nagasaki, Japan. Some of the better-known nuclear accidents occurred in 1986 at Chernobyl, 1979 at Three Mile Island, and, more recently, in 2011 at the Fukushima Daiichi Nuclear Plant, all of which happened at nuclear power plants. Nuclear releases pose some of the most effective measures for inflicting mass casualties and are the subject of numerous emergency planning measures throughout the world.

3.2.5 Explosive

Improvised Explosive Devices (IEDs) are explosive weapons carrying conventional, nonradioactive materials with the primary intention of inflicting harm on a subject. Commonly used as a warfighting or suicide bombing tactic, IEDs are sometimes deployed by terrorists to injure soldiers and other individuals. The 2013 Boston Marathon bombing and the 1995 Oklahoma City bombing are primary examples of intentional explosive events. Various accidental explosions occur occasionally, which may lead to homeland security concerns.

3.3 Stages of an Emergency Response

Most disasters occur at the local level, requiring municipalities to be prepared for a wide range of scenarios. If a local jurisdiction does not have the proper resources to respond to a disaster, state or federal government assistance may be required. These efforts must be escalated by a state's governor, who then applies to the President for federal relief. Under the Federal Response Plan (FRP), the Federal Emergency Management Agency (FEMA) coordinates and activates the response effort with collaboration from the appropriate federal agencies. Regardless of the degree of emergency, FEMA states that emergency management is generally broken down into four phases: 1) mitigation, 2) preparedness, 3) response, and 4) recovery, although adherence to the four stages is not a state-level requirement for grant funding (FEMA 2010). Mitigation and preparedness occur before or in anticipation of a release scenario while response and recovery ensue during or after the event.

While every emergency response effort is somewhat different, a similar structure for developing and maintaining plans for emergency operations should be kept standard. The federal government uses a five-category emergency response framework approach that differs slightly from the standard emergency management process. In 2011, the *Presidential Policy Directive 8: National Preparedness* (PPD-8) replaced the *Homeland Security Presidential Directive 8* (HSPD-8) and was intended to be a federal level guide on how the nation can prevent, respond to, and recover from homeland security threats (Lindsay 2012). The HSPD-8 establishes five emergency management frameworks that are intended to assign roles to various federal agencies fitting mission-specific areas (Lindsay 2012). The five frameworks are: 1) prevention, 2) protection, 3) mitigation, 4) response, and 5) recovery, and are expanded in this section. This report uses the five frameworks when referring to stages of an emergency response. Dispersion modeling may therefore occur at any stage of the response and provide vital decision-making guidance caused by the effluent release.

3.3.1 Prevention Framework

The key to preventing an emergency scenario from occurring in the first place or to minimize its disastrous effects is to practice mitigation activities (FEMA 1998). In the general emergency management sense, these activities include taking actions to reduce the chance of the impact of an emergency on human life, property, and the environment, including short- and long-term exposure effects. These activities ensure individuals and authorities are trained and prepared to handle an emergency before it happens, which includes establishing evacuation plans, stocking up on food and supplies, and planning how to respond and rescue lives (FEMA 1998). The National Prevention Framework assigns roles and responsibilities to federal agencies to help prevent imminent terrorist threats (Brown 2011). It helps coordinate information sharing and intelligence among agencies and assists in detecting terrorist threats

before they occur. The DOD and DHS have many specific roles related to the surveillance, prevention, and detection of potential terrorism and WMDs.

3.3.2 Protection Framework

The National Protection Framework provides guidance on how to secure the country against homeland security threats from acts of terrorism or natural disasters (Brown 2011). This would include the defense against WMD threats, critical infrastructure protection (including transportation, utilities, and agriculture), border security, and cybersecurity (Brown 2011). This framework relies on the coordination of existing capabilities to protect the homeland.

3.3.3 Mitigation Framework

The National Mitigation Framework presents a risk management strategy to reduce the loss of life, property, and impacts following natural or manmade disasters (Lindsay 2012). Since mitigation exists at all levels of the emergency response process, and most notably at the local level, some examples of mitigation efforts might involve: the procurement of insurance policies to mitigate financial impacts, retrofitting building structures to withstand severe weather or external conditions and making informed decisions on where to build or how to design structures (FEMA 2010). The federal National Mitigation Framework establishes large scale risk reduction strategies, initiatives to improve homeland resiliency, and efforts to reduce future risks (Brown 2011).

3.3.4 Response Framework

Immediately following the manmade or natural disaster, the response stage puts any preparedness plans into place and encompasses actions that are taken to save and sustain lives, reduce the loss of property, and support critical infrastructure after the incident has occurred (FEMA 2010). The National Response Framework provides a foundational guide informing how the country will respond to all types of disasters and emergencies by initiating the flexible National Incident Command System (ICS) and then aligning roles to various federal agencies (Brown 2011). If federal emergency response support is approved through a presidential order, FEMA will organize the response through its partner government agencies through the FRP and deploy individuals following ICS. This framework closely mimics the deployment and mobilization of emergency first responders such as firefighters, police, and medical services. External response support will also be activated in local, regional, or federal emergency operations centers (EOCs) to coordinate and direct logistics for those deployed in the field.

3.3.5 Recovery Framework

After the immediate danger of the episode has passed, the National Recovery Framework encompasses the short- and long-term efforts of rebuilding, restoring, and bringing the affected area back to pre-disaster conditions or better (Brown 2011; FEMA 2010). Depending on the situation (such as Hurricane Katrina in New Orleans), the recovery stage could take years, or the affected area may never be fully remediated. Recovery may also happen concurrently with response efforts. Specific efforts include rebuilding critical infrastructure, providing housing to survivors, restoring community services, and promoting economic development (Brown 2011). During a federal emergency response activation, EPA may be deployed for certain spills or releases that pose risks to human health and the environment

(more details are presented in **Section 3.6**). EPA is generally involved with the recovery and remediation phases of an emergency response since EPA is not a first-responding agency.

Three important components within the remediation role of consequence management are: sampling, decontamination, and waste management (Mikelonis et al. 2018). These areas are typically where the remediation methodologies developed within EPA's HSRP are implemented. Sampling is first conducted by air monitors or surface-based methods through vacuuming or swabbing (Calfee et al. 2013), which is time-consuming and expensive. Predictive modeling of atmospheric dispersion or stormwater runoff (Mikelonis et al. 2018) may be used to inform sampling locations. Decontamination methods such as spraying, fogging, or washdowns are then employed to mitigate the effects of the hazardous material (Ryan et al. 2010). Decontamination approaches can lead to large amounts of contaminated byproducts from supplies and personal protective equipment (PPE), along with the waste generated from the actual disaster. Effective waste management is the final critical component in the recovery phase to minimize contaminant exposure and remediate the affected area (Boe et al. 2013).

3.4 Operational Dispersion Modeling and Reach Back

Historically, the first dispersion models were developed to design control strategies for air pollutants released from industrial exhaust stacks (Beychok 1979). The development led to the implementation of dispersion models in the federal government for regulatory use in new stack construction or compliance with air quality standards such as the National Ambient Air Quality Standards (NAAQS). However, dispersion modeling was also found to be a useful, multifaceted scientific tool to inform public officials during accidental or intentional environmental releases, particularly due to their fast run times. Dispersion modeling for both regulatory and emergency response applications are part of the analyses and planning required by the Clean Air Act (CAA).

During times of crisis, first responders (local firefighters and police) are usually the first on the scene, typically within fifteen minutes of notification. Guidance information for evacuation and sampling is often needed within thirty minutes of a release, when containment is most critical (van de Walle and Turoff 2008), while other key decisions are generally made within one hour. To take advantage of dispersion model results, this timeframe would require emergency responders to 1) have the necessary knowledge to run a dispersion model, and to 2) know most of the physical details of the release and atmospheric parameters, as well as the model domain and boundary conditions. Local meteorology and release-source strength (mass of the release per unit time) are some of the most important components to initialize a dispersion model (OFCM 2002), in addition to secondary sources caused by the trapping and re-release of material in the wake of obstructions, leading to critical variations in contaminant concentration over short distances (Coceal et al. 2014). These variables are usually not known immediately and could introduce significant bias into the modeling results.

Since emergency responders generally do not have time to setup, run, and process results from a dispersion model, operational modeling options are available for large-scale and potentially high-impact situations when time is critical, and a modeled plume cannot feasibly be generated without external assistance. These operational modeling services are dubbed as "reach back" support, which is known in the military as the opportunity to reach outside a unit's traditional information flow to obtain additional intelligence and remain well-informed on specific matters (Radzikowski 2008). This section explains those choices, as well as federal reach back responsibilities and then identifies EPA's connection to dispersion modeling for emergency preparation and response.

3.4.1 Interagency Modeling and Atmospheric Assessment Center (IMAAC)

To provide a single point for the coordination and dissemination of hazard prediction products during an actual or potential incident involving federal government coordination, DHS established IMAAC as part of the National Response Framework (NRF; U.S. Department of Homeland Security 2016) to prepare and provide a more unified Federal response to disasters and emergencies. Currently led by FEMA, IMAAC is a collaboration between seven federal agencies, including DHS, DOE, DOD, NOAA, EPA, Nuclear Regulatory Commission (NRC), and the U.S. Department of Health and Human Services (DHHS), each with its own responsibilities for atmospheric plume modeling or a support role. IMAAC was formally recognized in April 2004 through a memorandum of understanding (MOU) through the Homeland Security Council Deputies Committee of DHS and is governed under the Homeland Security Act of 2002 for DHS to respond to and prepare for natural and manmade crises. FEMA assumes a key role in IMAAC under the Post-Katrina Emergency Response Management Reform Act of 2006 to prepare, plan, respond, recover, and mitigate effects to key infrastructure and resources following catastrophic incidents.

One of the primary reasons for IMAAC's creation was the inability of some federal agencies to properly coordinate dispersion modeling efforts. A noteworthy example occurred during the 1999 National Top Officials Exercise (TOPOFF) when various modeling systems produced confusing and contradictory results (US GAO 2008). TOPOFF2, a five-day full-scale simulated exercise, was intended to realistically test federal, state, and local emergency response systems should a high-profile CBRNe situation occur. During the exercise, dispersion models produced conflicting results because actual and mock meteorological inputs were used by different modelers without prior discussion. The resulting dispersion plumes, which were meant to inform emergency responders and the general public of potentially affected areas following a hypothetical release scenario, had the plumes impacting two different areas: one over the Pacific Ocean and another over the city of Seattle. The dispersion plumes led to an embarrassing appearance by the Washington State governor on television and ended with blame being placed on top officials for the misunderstanding (Mongeon 2018). The goal of IMAAC was therefore to provide a single official government dispersion prediction using the best possible government resources to lessen the chances of a repeated embarrassing scenario and to deliver the information more efficiently to first responders.

When requested by any state, local, federal, or tribal agency, IMAAC will organize a rapid, around the clock Federal response to produce a simulated atmospheric dispersion model plume. These products can be used by first responders to make informed decisions following an actual or potential hazardous release scenario. Plumes can be requested by email or through the Homeland Security Information Network (HSIN) helpdesk (phone number: (703) 767-2003) under significant real-world emergencies. IMAAC can also provide dispersion plumes for planning scenarios or national exercises, but a planning request will not take priority if another situation requires immediate attention.

IMAAC was also developed to support emergency responders in field response efforts. Following a hazardous release, the three primary questions from emergency personnel typically are: 1) when and where the greatest impacts could occur, 2) which areas are confidently out of danger from exposure, and 3) how long the response and remediation efforts could take. IMAAC results can be disseminated to emergency responders in as little as 20 minutes after the request with simple information such as where, when, and what was released. This preliminary information can provide the initial best guess needed to identify regions in the hot zone. The first model predictions tend to overestimate the actual event because details of the source characteristics are rarely known in emergency situations (OFCM 2002). The model results are then refined as additional information is reported from the scene.

Another justification for IMAAC was to reduce confusion over who should perform modeling in emergency situations and which models should be chosen. While IMAAC was not intended to replace agency-specific dispersion modeling activities, no permanent IMAAC dispersion provider has been officially identified. Instead, IMAAC fulfills its mission by providing a variety of dispersion resources through reach back support, where agencies or centers with specific scientific expertise (e.g., chemical, nuclear, biological) become activated and assume operational responsibility (Dadosky 2010). These agencies establish a baseline set of dispersion models that are regularly implemented and improved through research and development initiatives. NARAC, operated out of DOE's Lawrence Livermore National Laboratory (LLNL), has been designated as the primary IMAAC emergency operational hub with round-the-clock staff support, modelers, nuclear experts, and radiological monitoring teams. Currently, NARAC is the default reach back option for radiological and nuclear events but may also provide airborne hazard predictions for chemical and biological releases (Nasstrom et al. 2007). The Defense Threat Reduction Agency (DTRA), the DOD's official Combat Support Agency (CSA) for countering WMDs, is the official technical reach back for biological and chemical agent releases.

3.4.2 Models Used in IMAAC Responses

NARAC employs a comprehensive suite of proprietary modeling systems that integrate multiple LLNL models during a radiological or nuclear incident. Source-term models are fed into rapid effectsprocessing models or NARAC's own three-dimensional (3D) atmospheric dispersion models. For most cases, NARAC will use the Atmospheric Data Assimilation and Parameterization Tool (ADAPT) model to construct 3D meteorology fields for use in the dispersion model, Lagrangian Operational Dispersion Integrator (LODI) (Nasstrom et al. 2007). NARAC simulates the input meteorology for ADAPT's initial conditions through basic parameters obtained from the National Weather Service (NWS), or if there is an ongoing atmospheric release that is expected to continue for an extensive period of time, a research-grade mesoscale weather prediction model called the Weather Research and Forecasting (WRF) Model may be used (Nasstrom et al. 2007). Through a Lagrangian stochastic Monte Carlo approach (which calculates an average based on a nearly Gaussian distribution of atmospheric turbulence), LODI then solves the 3D advection-diffusion equation to produce a rapid and detailed plume within 5-15 minutes.

IMAAC reach back through DTRA uses the Hazard Prediction and Assessment Capability (HPAC) dispersion model suite. The main dispersion code for HPAC is built upon the Lagrangian Secondorder Closure Integrated Puff (SCIPUFF) model but has many advanced capabilities, including atmospheric transport and dispersion calculations, urban parameterizations, deposition, dose, and human effects-hazards. Real-time meteorology from the NWS is automatically pulled in through DTRA's meteorological data servers, which also host worldwide numerical weather predication (NWP) products from climate reanalysis data such as the National Centers for Environmental Prediction (NCEP) or the North American Model (NAM). These products can also be used to initiate WRF. HPAC's stochastic, second-order closure Puff model ensures that computations take only a few minutes, and an initial response can be sent to the requestor within 20 minutes.

Other advanced dispersion models such as Los Alamos National Laboratory's (LANL's) Quick Urban Industrial Complex (QUIC) model (Nelson and Brown 2013) are not part of IMAAC since QUIC lacks the integration of the SCIPUFF dispersion model. If EPA or NOAA is activated based on release type (such as inland oil spills), either agency may use the relatively simple co-developed CAMEO/ALOHA (Computer-Aided Management of Emergency Operations/Areal Locations of Hazardous Atmospheres) model (see **Section 8.6**), which is already used by many emergency responders. Dose projections for atmospheric radiological releases could be calculated by NRC's Radiological Assessment System for Consequence Analysis (RASCAL) model. The progression of radiological releases in nuclear reactors may be calculated through the MELCOR Accident Consequence Code System (MACCS) code. A summary of IMAAC agency responsibilities and models typically used for each release type is shown in **Figure 1**. More detailed information on each of these models will be presented later in this report.



Figure 1: Summary of IMAAC's agency responsibilities with the typical dispersion model used, based on information from DTRA (Runyon 2017).

3.5 Hazardous Release Mitigation Programs and Risk Evaluation

3.5.1 Emergency Planning and Community Right-to-Know Act (EPCRA)

EPA's chief responsibility is to act as a regulatory agency for environmental and human health concerns. Created in response to the hazardous methyl isocyanate release in Bhopal, India, EPA's Emergency Planning and Community Right-to-Know Act (EPCRA) establishes requirements for federal, state, and local governments to report on hazardous chemicals and increase public knowledge of the hazards in their local community. EPCRA contains four major provisions, including emergency planning, release notification protocols to the public, chemical storage reporting requirements, and a toxic chemical release inventory (EPA 2017). EPCRA's hazardous chemical inventory contains Tier I and II chemicals defined by the Occupational Safety and Health Administration (OSHA). Dispersion models may be used to inform EPCRA guidelines, but community planners are required to perform hazard analyses using "The Green Book" (EPA et al. 1987) to calculate threat, vulnerability, and screening zones around chemical facilities or storage areas.

3.5.2 EPA's Risk Management Plan Rule

The Federal government has mandated all facilities that possess, manufacture, and handle certain quantities of distinct regulated hazardous chemicals to develop risk and contingency plans should a harmful environmental release occur. To identify the potential effects of a chemical accident, document methods for hazard prevention, and establish emergency response procedures, facilities with hazardous substances must develop a Risk Management Plan (RMP) that is submitted to the EPA and revised every five years (40 CFR, Chapter I, Subchapter C, Part 68). The RMP rule was developed in response to the 1990 CAA Amendments (section 112(r)) so regulatory guidance is available to prevent chemical accidents

and expedite remediation. The RMP rule considers the use, storage, manufacturing, handling, or movement of an extremely hazardous substance at a stationary source site based on an extensive list of regulated chemicals (EPA 2009a). A facility's RMP must include several elements based on the type of program or processes that occur at the site. Generally, all facilities must include a description of the site and its regulated substances or processes that occur, the five-year accident history, the hazard assessment for the process, the potential worst-case scenario, and any site-specific emergency response programs should there be an environmental release (EPA 2009b).

A key element of an RMP is completion of a hazard assessment of the potential impacts from a release at the facility – effectively called an offsite consequence analysis. EPA provides guidance for this consequence analysis in EPA (2009c), which requires two elements: a worst-case scenario release and an alternative release scenario (i.e., the effect of a hypothetical accident under more realistic circumstances) (EPA 2004). The EPA guidance document offers several methods to carry out this analysis, including the use of dispersion models. However, the guidance is optional if the methodology or models can be substantiated (EPA 2004). The simplest guidance relies on lookup tables to provide conservative estimates of downwind risk and does not require computer modeling. More accurate site-specific consequences could be generated through dispersion model, fire or explosion model, EPA-established model, or another computational method (EPA 2009c). EPA's RMP*Comp dispersion modeling tool is one option that can be employed and is discussed in more detail in **Section 3.6.2**.

3.5.3 BioWatch

The mechanism, location, and timing of a chemical, radiological/nuclear, or explosive release may be possible to pinpoint (and thus remediate, model, evacuate residents, and decontaminate). However, biological vectors are often more challenging. Bacteria, spores, and other biological agents may be passively dispersed through the air or from person to person. During the 2001 Amerithrax events, it was unclear when, where, and how any further biological releases could occur. As a result, the DHS launched the BioWatch program in 2003 with the primary goal of detecting the presence of bioterrorism agents in large, densely populated urban areas. Deployed as a series of samplers, typically adjacent to the EPA's air quality monitors or in high human-traffic indoor and outdoor locations, the BioWatch program is the nation's first early warning system to detect certain known biological threats (NAS 2018). While the premise of the program is beneficial, it has received criticism for its monitoring methodology and high false-alarm rate. The BioWatch program does not operate any real-time samplers and therefore has minimal value for first responders seeking to obtain real-time information on biological pathogens (US GAO 2008). The only way to determine the presence of a harmful agent is to analyze the filter sample by completing a full laboratory analysis, which may take 24 hours or more after the sample is collected (NAS 2018). If a sample tests positive for any of a suite of biological agents, a BioWatch Actionable Result (BAR) is created and can trigger federal, state, and local response through the means of teleconferences and potentially the activation of a consequence management plan (e.g., sampling, public communication, environmental surveillance, event reconstruction) (NAS 2018). More than 50 BARs have been generated since the program's inception, but all have been false alarms due to naturally occurring organisms in the environment (NAS 2018). These BARs have led to mixed response and criticism for the program.

Even though LANL is not part of IMAAC, an around-the-clock modeling team may be activated directly by the BioWatch program if a noteworthy BAR is detected. LANL's BioWatch Event Reconstruction Tool (BERT) is run to simulate source inversion (determining a source location and strength based on dispersion modeling) or forward plume calculations. The QUIC dispersion model has also been employed to simulate biological releases for special events where BioWatch detectors are deployed. The future goal is to link QUIC with Argonne National Laboratory's (ANL's) Below Ground

Model so below- and above-ground biological-agent transport and dispersion can be captured and simulated (Michael Brown, personal communication, 2018).

3.5.4 Chemical Facility Antiterrorism Standards Program

The nature of certain facilities such as industrial chemical plants producing and using hazardous materials, power plants, or storage facilities makes them high profile targets for potential sabotage or accidental releases. To identify and help prevent and mitigate chemical releases from these types of highrisk facilities, the DHS has developed the Chemical Facility Antiterrorism Standards (CFATS) program. The purpose of CFATS is to identify and regulate high risk facilities to ensure that security measures and contingency plans are in place to reduce the effects of a terrorist-related attack associated with TICS. More than 300 chemicals, manufactured at plants that produce certain quantities, have been identified and must be regulated by CFATS. Based on the level of potential impact, CFATS focuses its efforts on the highest risk facilities and then employs a risk-based tiering system (6 CFR, Chapter I, Part 27). For example, any site that possesses more than 10,000 pounds of anhydrous ammonia must comply by reporting their holdings to the DHS CFATS program. The importance of the CFATS program for the interests of this report is that established, physics-based dispersion models may be used as part of the risk analysis methodology instead of employing EPA's RMP*Comp dispersion tool (81 CFR No. 71). Potential release scenarios could be run by IMAAC for planning initiatives, although DHS does not disclose what types of dispersion models might be employed. The CFATS program is important for EPA emergency response efforts in that it identifies these high-risk facilities, tiers their potential impact, and provides an inventory on the amount of hazardous TIC present should an incident occur.

3.6 EPA's Contributions to Emergency Response Initiatives and Dispersion Modeling

A wide-area CBRNe incident undoubtedly causes large-scale human safety, environmental, infrastructure, and economic concerns. If a local or state jurisdiction does not have the appropriate resources needed to respond to an emergency, federal emergency response may be required. In this capacity, FEMA is responsible for coordination and activation of the FRP. Response to wide-area incidents requires coordinated, multiagency approaches. Under the Homeland Security Presidential Directive 10 (HSPD-10), DHS coordinates with the appropriate federal agencies to respond to homeland security incidents. Before, during, and following natural disasters, terrorist attacks, or accidental emergencies, the federal government may enact a Continuity of Operations Plan (COOP) to sustain operational order. While the federal government has a series of eight National Essential Functions (NEFs) to continue leading the country during times of hardship, each agency is responsible for its Primary Mission Essential Functions (PMEFs). The EPA has one PMEF: to prevent, limit, and/or contain chemical, radiological, biological, oil, and other hazardous contamination incidents and provide environmental monitoring, assessment, and reporting for the incident. As a result, the EPA may act as the primary agency responsible for organizing the event with on-scene actions and local governments, or in some capacity to be the lead federal agency (LFA). These responsibilities are outlined under the DHS National Response Framework (U.S. Homeland Security 2016). In most cases, the EPA is LFA when the response is related to the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA: Superfund), EPCRA (planning for chemical emergencies), the Clean Water Act, the Safe Drinking Water Act, the Oil Pollution Act, the CAA, and the Resource Conservation and Recovery Act (RCRA: hazardous and general solid waste disposal). Additional responsibilities involve the cleanup of impacted buildings or natural areas, recovery from terrorist attacks or natural disasters, and support to drinking water systems.

For initial radiological and monitoring assessments, the DOE is generally considered the LFA, but EPA would assume intermediate and long-term response once the initial threat has subsided (U.S.

Homeland Security 2016). EPA would also be the LFA with accidents involving shipments of radiological materials not licensed or owned by a federal agency, as dictated by the Federal Radiological Emergency Response Plan (FRERP). When EPA is the LFA, on-scene coordinators (OSCs) assume the position of the lead federal officials. At the site level, EPA's OSC personnel assess, monitor, and control the response with the incident command and employ research developed by scientists in the agency (Mikelonis et al. 2018) to streamline the response process.

Even though EPA is not technically a first-responding agency as opposed to local or regional police, fire, and emergency medical service (EMS), dispersion modeling may play an important role in agency actions after EPA assumes responsibility at least 72 hours after the release. Various tools and strategies such as predictive computer modeling can be employed to protect human health and the environment and respond to wide area incidents (Mikelonis et al. 2018). These plume predictions could help guide field sampling efforts, and the sampling results could then be used to update the plume and refine estimates. The dispersion models developed, used, and improved by the EPA are expanded in the following sections.

3.6.1 EPA Support Center for Regulatory Atmospheric Modeling

EPA implements dispersion and predictive modeling tools for regulatory applications, emergency preparation and response, and research and development purposes. EPA's Support Center for Regulatory Atmospheric Modeling (SCRAM) website provides public access to air quality and dispersion models and resources developed by the agency. SCRAM also delivers training and resources, reports and journal articles, and other modeling guidance. The EPA has also established a list of agency-preferred and recommended models for screening purposes, state implementation plans (SIPs), and downwind calculations from source to receptor for regulatory and permitting use (Appendix W 40 CFR part 51). The models identified as preferred agency options are assessed for quality assurance so that criteria are met for scientific rigor, model development and evaluation, peer reviewed theory, and the ability to provide transparent, reliably disseminated information (www.epa.gov/quality). Some of EPA's preferred and recommended dispersion models, all of which are Gaussian plume models, are AERMOD (American Meteorological Society/Environmental Protection Agency Regulatory Model; Cimorelli et al. 2005; see Section 8.5), CTDMPLUS (Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations), and OCD (Offshore and Coastal Dispersion Model). These models are identified later in this report, but only AERMOD is expanded in further detail since these models are not generally used for emergency response. EPA also suggests alternative and screening models on the SCRAM website for other applications.

3.6.2 RMP*Comp

As part of the EPA's RMP rule, the agency provides resources to chemical facilities so they can develop their site-specific consequence analyses. The facilities may employ their own public or proprietary dispersion model of choice if they are willing to share the results, the model is recognized within the industry, the model is applicable for the chemical release being simulated, and it defines the appropriate parameters and worst-case scenarios (EPA 2009c). However, EPA also provides a free, web and desktop computer-based RMP*Comp dispersion modeling tool, which was co-developed by EPA and NOAA. The program incorporates database tables of regulated materials including 77 acutely toxic substances and 63 flammable gases and volatile liquids. Based on the amount released, RMP*Comp determines the downwind distances to an endpoint location for probable and worst-case scenario events for standard atmospheric temperatures (25°C), low winds (1.5 m/s), and stable conditions (stability class F). The program can handle vapor cloud fires for flammable gases that are liquefied under pressure (EPA

2009c). However, RMP*Comp is not a model to be used for emergency response as it only allows the user to select the amount released, liquid temperature or chemical physical state, and sometimes the surrounding terrain type. Moderate ambient air temperatures, low-to-moderate wind speeds, and stable atmospheric conditions are assumed during the planning scenario, which does not always reflect the atmospheric state during an actual release, potentially lofting the chemical or allowing it to travel farther downwind.

3.6.3 CAMEO/ALOHA

RMP*Comp is meant to easily plan and identify high-priority hazards for an RMP, but more sophisticated co-EPA-developed modeling tools are available for emergency response use such as the CAMEO Software Suite. CAMEO (also see **Section 8.6**), which includes four distinct entities: 1) CAMEO Chemicals, 2) CAMEO*fm*, 3) ALOHA, and 4) MARPLOT. CAMEO Chemicals is a comprehensive, proprietary database of hazardous chemical datasheets and physical properties, which provides information similar to the information seen in the classic orange US Department of Transportation (DOT) Emergency Response Guidebook (ERG). The ERG is still a go-to resource for most first responders, as it provides basic guidance to determine the extent of a and its approximate evacuation distances (Christine Wagner, personal communication, 2018), as well as chemical releases since results are generated within seconds from only a few details about the release and current meteorology. ALOHA was first developed by EPA and NOAA in the late 1980s specifically for use by first responders, including EPA's Environmental Response Team (ERT). The plotting software in CAMEO is MARPLOT. The entire CAMEO software package is available as a free download for laptops and mobile phones from NOAA's Office of Response and Restoration.

ALOHA is identified in this section because it can also be used to perform RMP guidance. Since ALOHA performs more sophisticated dispersion analyses due to specific and refined input parameters, it may provide results that do not closely match RMP*Comp. However, ALOHA cannot be used to inform EPCRA hazard analyses because the quick and simple calculation methodologies in EPA et al. (1987) (i.e., "The Green Book") are used instead. The Green Book capabilities are available in the CAMEO*fm*, which is used to manage planning data such as details about a particular facility, chemical transportation routes, and emergency response procedures about chemicals in a local community. The Green Book may also provide results that do not closely match ALOHA due to its simplifying assumptions. While also simplified, ALOHA can account for different atmospheric stabilities, dispersion parameters based on terrain, temperatures, liquid evaporation rates, and buoyant or dense gases (Jones et al. 2013).

4.0 Atmospheric and Micrometeorological Fundamentals in Dispersion Modeling

The purpose of this section is to outline fundamental components of boundary layer meteorology and micrometeorology (meteorological processes on a spatial scale of \sim 1-10 km and a temporal scale of \sim 1 hour to 1 day) that dictate the transport and dispersion of a hazardous release. This section is not meant to be a comprehensive explanation of PBL processes, but more of a resource to introduce salient concepts employed within dispersion models. More in-depth explanations of micrometeorology and its associated processes are covered in Stull (1988) and Arya (2001; 1999). Dispersion models simplify the complex atmospheric state by using equations that govern the dispersion of pollutants under the assumptions of stationarity and horizontal homogeneity, frequently based on Gaussian downwind concentration patterns. However, the atmosphere is very turbulent, especially close to the ground surface where roughness elements (e.g., trees, buildings, vegetation, topography) create complex and variable flows, and physical variables (due to solar heating, moisture, and the overall large-scale atmospheric state) are in constant flux. Since the fate and transport of contaminants is significantly influenced by turbulent exchange in the PBL, the fundamental concepts are introduced here. This section satisfies Objective 4 as described in **Section 2.3**.

4.1 Atmospheric Turbulence

The dispersion (transport and diffusion) of atmospheric contaminants is strongly influenced by microscale physics. While pollutant transport is primarily a function of the mean wind, small-scale atmospheric turbulence is the fundamental driver of plume dispersion. According to Arya (2001), atmospheric turbulence is defined as the highly irregular, random, and almost unpredictable chaotic fluctuations of wind velocity, temperature, and scalar concentrations around their mean values. The irregular fluctuations in a turbulent flow are functions of time at fixed points in space. Turbulence occurs in the PBL where the earth's surface strongly influences small scale motion, temperature, water vapor, and pollutants. Turbulent flow constantly undergoes random changes in both magnitude and direction, visualized as irregular vortex-like swirls of motion called eddies. These vortices are not clearly defined structures or features, but more of a concept to qualitatively describe turbulence on the order of 0.001 m to 1000 m in diameter in the PBL (Stull 1988). Turbulence consists of many different eddies superimposed on each other where the strengths of eddies of various scales define the turbulence spectrum. However, turbulence is not as easy to precisely define, as certain wave motions in the atmosphere may be irregular and chaotic but not necessarily turbulent.

Useful rules of thumb to describe atmospheric turbulence can be defined by the five following criteria provided by Arya (2001) where the flow is:

- 1. <u>Irregular and random</u>: These motions make turbulence <u>nearly</u> unpredictable and irreproducible, meaning that a statistical description of turbulence must be employed (i.e., wind fluxes are described by means, variances, fluxes, etc.).
- 2. <u>3D and rotational</u>: Three-dimensional velocity fields and the presence of vorticity or rotation that are highly variable in space and time.
- 3. <u>Ability to mix</u>: turbulent diffusivity is responsible for the dispersion and spread of pollutants in the PBL and is also effective at exchanging momentum and heat. This is often regarded as the most important property of turbulence.
- 4. <u>Ability to dissipate</u>: turbulent motion is continuously dissipated and turned into heat or internal energy by viscosity, meaning that turbulence will decay if it is not produced continuously.
5. <u>Multiple scales of motion</u>: turbulent flows contain a wide range of scales, and the ability to transfer energy from one scale to the other is important and key to larger atmospheric processes.

Turbulent eddies create fluctuations in wind velocity, temperature, humidity, and scalar concentrations causing their components to vary irregularly in time or space around their mean quantities. This can be thought of as a fluctuating component superimposed on the mean quantity. The basis of Reynolds averaging (Reynolds 1894) for wind describes the wind's components (u, v, and w for longitudinal, lateral, and vertical, respectively) consisting of their characteristic mean (\bar{u}) and fluctuating (u') portions, called Reynolds decomposition. Many meteorological applications use average wind over time, but in dispersion modeling, the fluctuating components are key considerations that point to the PBL's vertical structure (Pasquill and Smith 1983). Simple Gaussian dispersion models may only require the wind speed and direction averaged over a longer time period. However, more complex models that track and simulate a puff or particle over numerous time iterations may benefit from the wind's fine-scale fluctuations.

4.2 Planetary Boundary Layer

Dispersion models are commonly used for multiple simulations over short durations (on the order of one-hour averages) and relatively small areas of spatial interest (< 20-50 km) in the atmospheric region closest to the earth's surface called the PBL. This 0.2-3 km vertical layer of atmosphere connects larger scale weather patterns (mesoscale: ~10s-100s of km, and synoptic: >1000 km) to those driven by surface-related effects (**Figure 2**). The PBL is a dynamic and constantly changing portion of the atmosphere that is influenced by terrain, vegetation, water bodies, heat and moisture fluxes, and human-introduced influences such as anthropogenic emissions, urban canopies, and alterations to the ground surface. The PBL varies diurnally based on solar heating and seasonality.

During the middle of the day, the PBL has typically grown to its thickest point due to surface heating from the sun and the formation of buoyant thermals. This daytime layer is referred to as the convective mixed layer (CML). The CML grows by entrainment, or the downward mixing of air from a more stable layer above. It begins to grow just after sunrise, reaches its maximum point during the day, and shrinks in height (collapses) by sunset. Conditions that include an unstable boundary layer and high air flow during the daytime hours (due to increased wind speeds, buoyancy, or turbulence) usually mean that a release will disperse faster than during the evening, although detrimental effects can be transported farther downwind.

As the sun slowly sets, solar heating to the surface is cut off and the PBL slowly transforms into a stable (nocturnal) boundary layer (SBL) nearest to the surface and a residual layer (RL) above. The RL is a neutrally stratified zone where turbulence exists from the previous day's CML and tends to be equal in intensity from all directions (Stull 1988). The SBL is characterized by stable atmospheric conditions (where vertical motions are suppressed) with light or calm winds and minimal turbulence directly above the surface. The lower part of the RL is transformed into the evening SBL due to its contact with the ground and radiational cooling. A capping temperature inversion usually develops above the RL. Air in the SBL is statically stable with the potential for intermittent weak turbulence (low-level or nocturnal jets), making the evening boundary layer perhaps one of the most difficult to predict in dispersion modeling due to complex transport, diffusion, and spurts of turbulence in combination with natural and anthropogenic surface effects (OFCM 2002). The increase in atmospheric stability and a general decrease in wind speed during the evening and overnight hours may mean that a release will disperse more slowly than during the day but also remain concentrated near the emission source.

As the sun rises in the morning hours, solar heating once again grows turbulence and starts to mix the two layers by entrainment and gradually builds the convective boundary layer, resulting in the entrainment zone extending to the surface as the SBL erodes. During all periods of the day and night, the surface layer (SL) is generally defined as approximately the lower 10% of the PBL and is a complicated area where turbulent fluxes, stresses, surface roughness, and other perturbations affect wind flow directly above the ground surface (Stull 1988). While the SL is arguably one of the most important regions for understanding pollutant dispersal, particularly at breathing levels after a release, it is also one of the most difficult to predict, simulate, or otherwise parameterize in dispersion models. Complex PBL relationships are often simplified when parameterized in dispersion models, which can translate into lower model performance. Specifically, complex terrain effects, coastal influences, and urban canopies introduce fine scale meteorological variations that complicate modeling efforts.



Figure 2: The common, but idealized, diurnal evolution of the Planetary Boundary Layer (PBL) adapted from Stull (1988).

The PBL is also significantly modified over urban areas due to increased roughness effects from the presence of buildings and other man-made landscape alterations. With lower surface albedo due to dark pavement, concrete, and lack of vegetation, as well as increased anthropogenic emissions, urban areas frequently result in localized regions of higher temperatures called the urban heat island (UHI) effect. This phenomenon results in higher overall temperatures both laterally and vertically around the urban area based on the density of buildings. The urban boundary layer (UBL) creates a gradient or "dome" of locally warmer temperatures in comparison to more rural locations, where a "cliff" or a steep rise in temperature is seen between the transition of rural to suburban locals, followed by a "plateau" over suburban portions of the outer city, and a "peak" over the city center (Oke 1988). Diurnal changes in temperatures may be a few degrees warmer due to the increase of incoming longwave radiation, as well as absorption and reemission by the polluted urban atmosphere (Arya 2001). A decease in surface albedo may cause a decrease in outgoing longwave reflection or shortwave radiation emission, causing a greater daytime heat storage and decreased evaporation. During clear skies and calm wind conditions, thermal modifications of the UBL tend to dominate over roughness effects created by the buildings (Arya 2001). As the boundary layer erodes during the evening and overnight hours, the UBL tends to decrease in altitude but remains higher than in rural locations where strong atmospheric stability suppresses turbulent vertical mixing.

The sections of the PBL are therefore not always homogeneous. When the approach flow is modified by changes in roughness or temperature differences over the surface, a change in the mean wind profile and turbulence may be seen near the surface. This modified layer is called an internal boundary layer (IBL) because it grows within another boundary layer associated with the approach flow (Arya 2001). Notable examples occur when there is a dramatic change of surface roughness where the flow suddenly moves between a grassy field to a stand of trees, from a water body to a shoreline (leading to land and sea breezes), or upon entering an urban area to a rural location.

4.3 Modifications to Urban Flow from Building Structures

While the UBL influences the local mesoscale flow regime, complex wind behaviors exist within the urban canopy. Buildings and streets alter the overall wind flow patterns and cause complicated turbulence that could disperse harmful pollutants and affect the exposure for urban inhabitants. In addition to the effect of industrial emissions on poor air quality, transportation-related emissions associated with vehicles and other releases have a large effect on localized urban air pollution. Especially under low wind conditions, buildings can restrict ventilation and keep localized concentrations of pollutants very high at breathing level or in isolated recirculation zones.

A street flanked with buildings on either side is classically referred to as a street canyon (Nicholson 1975), although some urban geometry may contain discontinuous street canyons with intersections and building breaks. The schematic in Figure 3 from Halitsky (1968), as described in Arya (2001), shows how the mean velocity profile and background flow become altered and separated when the windward end of the building is encountered. In the lower portion of the UBL, flow on the windward side of the obstacle creates a clockwise turbulent eddy due to pockets of low pressure and reversed flow at various locations around the building (Monbureau et al. 2018). Once the flow is forced up and over the building, high turbulence intensity and reverse flow form a recirculating "cavity" zone on the lee side of the building (Monbureau et al. 2018), which may bring contaminants to the street surface and lead to downwind stagnation, especially when the mean wind speed is < 1.5 m/s (DePaul and Sheih 1986). This effect can entrain outside pollution and/or accumulate contaminants emitted inside the cavity, leading to high concentrations as wind speeds remain low but wind shear and turbulence intensity is high (Arya 2001). The size of the cavity depends on the length, width, and height (L_b, W_b, H) of the building or obstacle, as well as the characteristics of the approach flow. The mean velocity profiles are also shown in **Figure 3b**, depicting the small counter-gradient flow in the cavity. The flow separation between the regions in the cavity and farther downwind are called the near and far wake regions, respectively. The far downwind wake is associated with enhanced turbulence intensity and negative vertical velocity as the flow begins to recover from the encounter with the building. Wind tunnel studies have shown that the influence of buildings and their wakes can extend to 10-20 building lengths downwind and beyond (Arya 2001). These flow separation effects occur as the fluid flow of the air attempts to transfer from high to low pressure to remain in equilibrium.

Figure 4 shows the influence of pollutant dispersion within an idealized symmetrical street canyon based on the findings of Dabberdt et al. (1973). Due to pressure and turbulence effects, some of the mean synoptically induced wind flow above the rooftops enters the street canyon and creates a localized vortex, thereby restricting the recirculation of anything that is emitted within. However, the aspect ratio (the average building height (*H*) divided by the street canyon width (*W_c*)) strongly influences street canyon flow. Street canyons tend to have aspect ratios $H/W_c \approx 1$, while wide avenue canyons could be below 0.5, with deep canyons > 2. Short, medium, and long length canyons can be characterized by their approximate length (*L_c*) divided by height such as $L_c/H \approx 3$, 5, 7, respectively (Vardoulakis et al. 2003). Wide canyons with $H/W_c \sim 0.3$ (**Figure 5a**) create an isolated roughness flow that develops a cavity directly in lee of the first upwind building and on the windward side of the second, but the center of the canyon may remain coupled with the mean flow. For wake interference flow when $H/W_c \approx 0.5$ (Figure 5b), the disturbed air does not have enough distance to modify its flow before encountering the next obstacle (Vardoulakis et al. 2003, Oke 1988). Finally, $H/W_c > 1$ results in skimming flow in the street canyon (Figure 5c), allowing the formation of a single vortex. Additional areas of low pressure and wind recirculation zones could occur on street corners or intersections. Low wind speeds and/or deep canyons with $H/W_c > 1$ may create recirculating cavities that leave the breathing level largely stagnant (Grimmond and Oke 1999). In addition, the presence of a taller building among shorter buildings, as well as the distance and orientation between them, can significantly modify the flow downstream (Arya 2001), as shown in wind tunnel experiments with a tall tower among an array of shorter buildings (Heist et al. 2009).



Figure 3: Schematic of a) cavity and wake flow zones associated with a building or other square obstacle in the mean flow and b) its relationship with the vertical wind profile, after Halitsky (1968).



Figure 4: Schematic of streamlines when perpendicular flow encounters a street canyon, based on Dabberdt et al. (1973).



Figure 5: Various perpendicular flows for urban canyons with a) isolated roughness, b) wake interference, and c) skimming flow aspect ratios, based on Oke (1988).

4.4 Vertical Wind Profile

A vital input to most atmospheric dispersion models is an accurate representation of the vertical wind velocity profile (the change in wind speed with height) just above the ground surface, as it will dictate how fast and far a pollutant disperses. As a general principle, mean wind speed typically increases with height because the effects of friction and surface roughness are lessened farther away from the ground surface. Two commonly used wind profiles in dispersion models are the logarithmic wind profile and the power law. The logarithmic wind profile or "Law of the Wall" is a semi-empirical relationship that depicts wind speeds close to the surface under well developed, neutral boundary layer conditions:

$$\bar{u} = \frac{u_*}{k} ln \left[\frac{z - d}{z_0} \right] \tag{1}$$

where \bar{u} is the wind speed at height *z*, u_* is the friction velocity, *k* is the Von Kármán constant (0.4), *z*₀ is the surface roughness length, and *d* is the zero-plane displacement due to obstacles. Ten meters is commonly used as the reference height to avoid surface-related effects. The logarithmic wind profile is generally applicable in the lowest several hundred meters of the PBL (Stull 1988). A simple alternative to the logarithmic wind profile is the power law expression:

$$\frac{\bar{u}}{\bar{u}_r} = \left(\frac{z}{z_r}\right)^m \tag{2}$$

where \bar{u} is the mean wind speed at height *z*, and \bar{u}_r and z_r are the reference wind speed at reference height, respectively. The exponent *m* is based on the type of surface and is approximately 0.1 for smooth surfaces and roughly 0.4 for urban areas (Arya 1999). The logarithmic wind profile (1) is commonly used in many dispersion models and is considered more effective than the power-law wind profile, and (2) is in the lowest 20 meters above the surface. Both methods provide a good estimation up to 100 m, but the power-law is then more appropriate above 100 m and in the lowest part of the PBL (Cook 1985).

The urban canopy boundary layer profile, another type of vertical wind profile used in dispersion models, is used for situations in which there are buildings upwind of a release source, and the user wants to account for urban drag on the inflow profile. The urban canopy boundary layer profile is not intended for large downtown high-rise structures. (M. Brown, personal communication, 2018). The formula represents vertical wind speed with height for two conditions: above and below H in the domain (where H is the average height of the urban building canopy). The urban canopy profile accounts for lower wind speeds below H as it is slowed by the drag from the buildings:

$$\overline{u} (z \le H) = \overline{u_H} \exp\left(A\left(\frac{z}{H}\right) - 1\right)$$
(3)

where $\overline{u_H}$ is the mean velocity measured at *H* and *A* is the attenuation coefficient representing the average impact of the buildings or vegetation canopy on the flow (Nelson and Brown 2013). This equation (3) was originally presented by Cionco (1965), who developed a wide range of empirical values for *A* (Cionco 1978). These values were introduced to modify flow based on vegetation canopies for a wide variety of grasses, shrubs, and trees. The values represent an altered airflow response to vegetation roughness and density, with values of approximately 1-2 for small trees, rice, and corn, and up to 4.5 for maple, fir, and gum trees. Lower values represent rigid and sparsely arranged objects, while higher numbers indicate dense and flexible obstructions (Cionco 1978). Buildings are undoubtedly dense as well as rigid, so there is not a widely accepted value for *A* since the equation was not intended for dense urban use.

At heights higher than H, a transition to a modified logarithmic wind profile is introduced:

$$u(z > H) = \frac{u_{ref} \left[ln \left(\frac{z - d}{z_0} \right) + \psi \left(\frac{z - d}{L} \right) \right]}{ln \left(\frac{z_{ref}}{z_0} \right)}$$
(4)

where *L* is the Obukhov length, which accounts for stability effects. Equation (4) is used to avoid discontinuities in the velocity profile (Nelson et al. 2009). The premise behind the equations is discussed in further detail in MacDonald (2000). Nelson et al. (2009) recommends setting z_{ref} equal to *H* (and therefore u_{ref} is the upwind velocity at *H*) to avoid the wind speed ballooning above the canopy height that may introduce erroneous results.

5.0 Types of Atmospheric Dispersion Models

Atmospheric dispersion modeling has evolved tremendously over the past 100 years while still retaining many of the theoretical and mathematical representations of the fundamental dispersion equations. Even though dispersion modeling has seen improvements throughout the decades, many of the mathematical foundations are still based upon the original building blocks of Gaussian dispersion models (i.e., Pasquill 1962, 1974), Lagrangian particle models (which track a particle or puff under a moving frame of reference), stochastic (random walk) or other statistically based models, or Puff models. By the 1960s and 70s, computers began to be commonly used to solve Gaussian plume equations rapidly instead of completing the computations by hand. As computers advanced in the 1980s, Lagrangian Puff models and simple Eulerian models (with a fixed frame of reference as particles are free to move throughout the domain) were introduced. The 1990s and 2000s saw an advancement of Eulerian 3D grid models as algorithms and model resolution improved. Today, higher-order CFD models are commonly used in research applications but are rarely used by emergency responders in the field. For this reason, classic and relatively simple Gaussian-based dispersion models continue to be at the forefront of emergency response due to their fast output times, although higher fidelity models are also used for emergency preparation exercises.

Dispersion and diffusion models predict the distribution and concentration of a constituent downwind and in a typical study, the local meteorological scenarios are defined in terms of a characteristic wind speed, direction, and atmospheric stability. The atmospheric state and stability (i.e., stable, neutral, or unstable/convective) may be represented by the discrete Pasquill stability class (Pasquill 1961), a function of wind speed, solar radiation, and cloud cover, as turbulence measurements are rarely available for the model domain of interest (Bowers et al. 1994). More recent advances in dispersion modeling parameterize atmospheric stability using Monin-Obhukov similarity theory (e.g., Cimorelli 2005). Models also require basic information on the amount of material released (source term) and removal mechanisms. The process components of a dispersion model are shown in the flow chart in **Figure 6**. The rest of this section provides a broad overview of the different types of dispersion models can be seen in **Figure 7**. The strengths and limitations of different types of dispersion models are also provided in **Table 1**. This section satisfies Objectives 5 and 6 as detailed in **Section 2.3**.

5.1 Box Models

These simple models assume that the domain is one large homogeneous volume, and any substance entering this volume is uniformly and instantly mixed throughout the box (Arya 1999). Box models are generally stationary (considering a city area or the transport between two regimes such as the troposphere and stratosphere) and may consider fluxes or flow in and out of the box (F_{in} and F_{out}), production (P), chemical loss (L), deposition (D), and emission (E) terms to understand production and destruction in simplistic terms (5). Box models can often be solved on paper through the addition or subtraction of production and loss terms and are best used for quick, simplistic transport calculations. The mass balance of a box model is the sum of the sources minus sum of the sinks:

$$\frac{dm}{dt} = \sum sources - \sum sinks = F_{in} + E + P - F_{out} - L - D$$
(5)



Figure 6: Components of an atmospheric dispersion model, modified after OFCM (2002) and Turner (1979).

5.2 Gaussian Plume Models

The Gaussian plume model is often used as the fundamental basis for many dispersion models and is particularly useful for quick calculations that assume conditions to be horizontally homogeneous. Most Gaussian plume models also imply that the pollutant source is released continuously and that the concentration profile downwind of the release has a cross-section that resembles the classic Gaussian bell-shaped distribution. The formulas are derived assuming steady-state conditions because their results represent ensemble averages. Since the model assumes that meteorological conditions will remain constant across the horizontal domain over time, a Gaussian plume model is best used for estimates within 20-50 km of the release location as long as the wind direction and speed are consistent. Therefore, it is essential that the source term characteristics be accurate for the best model results. Gaussian plume models are challenged in urban areas with complex building geometries because localized releases interact with street canyons and building wakes, especially in the near-field region close to the release point (Belcher et al. 2013). Comprehensive field, model, and laboratory understanding are generally lacking for near-field dispersion effects (Coceal et al. 2014).

Early solutions to the diffusion equation implemented in basic Gaussian diffusion models were based on turbulent transport of material through the gradient transport theory or the "K-Theory", in which models assumed that turbulent transport was proportional to the gradient of the mean concentration, and a proportionality factor, or diffusivity, was implemented to represent turbulent transport. Boundaries usually play a large role in dispersion, including the presence of a temperature inversion or interaction of the plume with the ground. Therefore, when the plume deflects off a surface, an "imaginary" source is represented using the modified equation by Turner (1970). The Gaussian downwind concentration (\overline{C}) at downwind distance *x*, lateral distance *y*, and vertical distance *z* for a continuous point source is represented as:

$$\bar{C}(x,y,z) = \frac{Q}{2\pi\bar{u}\sigma_y\sigma_z} exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \left\{exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\}$$
(6)

where Q is the source strength, or emission rate of the released material, usually in grams or milligrams per second; \bar{u} is the mean transport wind speed in meters per second, which usually represents the wind at source height or the layer containing the plume; and $\sigma(x, y, z)$ is the longitudinal (along-wind), lateral (crosswind), and vertical dispersion coefficients in meters, which may be based on the classic Briggs (1973) equations or the Pasquill-Gifford-Turner (PGT) stability classes and curves (Gifford 1961; Pasquill 1961; Turner 1970) and other formulations, and H accounts for the source release height. Arya (1999) and Bowers et al. (1994) expand on these equations in much more detail, and a complete set of Gaussian plume equations for various sources (such as line, point, or area sources that contain continuous releases) is provided. Examples of Gaussian Plume models are AERMOD (see **Section 8.4**) or ALOHA (see **Section 8.5**).

5.3 Gaussian Puff Models

This model type (also known as a segmented plume) divides the emission into a series of overlapping "puffs", allowing the release source no longer to be steady, if desired. The horizontal meteorological conditions also do not need to be homogeneous. Puff models may treat releases as point, line, or area sources where a pollutant is released as one instantaneous amount (as in an explosion) and then tracked with the Eulerian or Lagrangian frame of reference. Puff models may also encompass a series of successive near-instantaneous releases or "puffs" that are released and tracked discretely into the ambient environment, since even continuous releases could be thought of as a series of overlapping puffs (Arya 1999). Each individual puff is simulated by numerically integrating the 3D advection diffusion equation as it diffuses into the air based on constant or time-varying wind conditions. According to the statistical theory of diffusion, the mean concentration of a puff is Gaussian in all directions (unless affected by an external barrier like a temperature inversion or obstacle), and the spread of the plume puffs is related to statistical diffusion parameters (Arya 1999). Each puff of material is assumed to be horizontally symmetrical and the average concentration (\overline{C}) in the puff follows the Gaussian form from Slade (1968):

$$\bar{C}(x, y, z) = \frac{Q}{(2\pi)^{\frac{3}{2}} \sigma_x \sigma_y \sigma_z} exp\left[-\frac{1}{2} \left(\frac{x}{\sigma_x^2}\right)^2\right] exp\left[-\frac{1}{2} \left(\frac{y}{\sigma_y^2}\right)^2\right] \\ \left\{exp\left[-\frac{1}{2} \left(\frac{z-H}{\sigma_z}\right)^2\right] + exp\left[-\frac{1}{2} \left(\frac{z+H}{\sigma_z}\right)^2\right]\right\}$$
(7)

The lateral plume dispersion parameter σ_y in the first denominator is assumed to be equal to σ_x as a simplifying assumption in the integrated plume method. The Gaussian Puff approach leads to calculations that could be more accurate since each successive puff responds to the overall wind conditions and is tracked across multiple sampling periods. Puff models can be used for chemical or radioactive releases and are better applied to continuous releases over a longer sampling period (instead of instantaneous). However, the plume shape may vary based on sampling time versus puff travel time from source to receptor (Hanna et al. 1982). Urban areas within the trajectory of a puff are often parameterized as roughness elements, so the effects of single buildings, clusters, or full cities are not generally captured. SCIPUFF is the main Lagrangian Gaussian puff dispersion code of the HPAC model commonly used through IMAAC emergency response (DTRA 2004).

5.4 Lagrangian Stochastic Particle Models

A Lagrangian model divides emissions into small particles or parcels that are tracked individually as they are stochastically transported and diffused downwind. At each time step in the model, the particles

are moved by 1) the mean wind, 2) turbulent diffusion by random fluctuations in the horizontal and vertical winds, and 3) molecular diffusion. The trajectories of particles in the 3D wind field are calculated by the random walk method. Lagrangian dispersion models are typically employed for incidents involving complex meteorology, strong wind shear, or complex wind schemes in urban areas (OFCM 2002). Since the trajectories of thousands (or millions) of particles are tracked on each model time step and based on the turbulent deviation of the wind from the previous time step, the simulation could be computationally intensive. However, meteorological variables including wind fields are often run "offline" from the dispersion code (i.e., not at the same time). Some researchers and operational modeling centers believe Lagrangian models such as NARAC's LODI model used in IMAAC (Bradley 2005) can resolve point sources and simulate turbulent diffusion in greater detail than Gaussian models. The QUIC model (Nelson and Brown 2013) is another example of a Lagrangian stochastic model, as well as NOAA's Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model that is widely used for long-range trajectory and dispersion calculations (Stein et al. 2015).

5.5 Eulerian Grid Models

In a Eulerian grid model, the domain is divided into a 3D array of rectangular grid cells where within each cell, the mixing of a substance is uniform and instantaneous. This type of model is best used to understand regional air quality issues such as ozone (O_3), particulate matter (PM), and nitrogen oxides (NO_x), and is more commonly referred to as a regional air quality or mesoscale atmospheric model, rather than a dispersion model, although they can be applied to regional dispersion. EPA's Community Multiscale Air Quality (CMAQ) model (EPA 2019) is an example of a Eulerian Grid model. Since these models are usually meant for larger spatial or temporal scales and regional air quality issues, they will not be covered in this document since this work is more focused on near-field dispersion.

5.6 Higher Order Models

Dispersion in complex urban environments often involves complex phenomena that lower-order dispersion models are unable to capture adequately. However, due to the dramatic increase in computational power over the past few decades, CFD model advancements using LES or Reynolds-averaged Navier-Stokes (RANS) methods can provide a more detailed description of the flow and dispersion surrounding complicated urban obstacles with varying geometries (Tominaga and Stathopolous 2013). Traditionally, CFD models have been useful for research, case studies, or emergency planning initiatives and are best applied to understand site-specific phenomena rather than for operational use due to their complex input data preprocessing requirements and longer computational times. In this capacity, reduced-order Gaussian dispersion models are still of prime significance due to their widespread use in operational settings and timely simulation results (Philips et al. 2013). However, CFD and LES simulations can provide denser evaluation datasets than field or laboratory studies and can be used to improve algorithms in other dispersion models.

CFD models portray the advection and diffusion of pollutants in a fluid flow. The transport of a contaminant is solved through the Navier-Stokes equations, which describe the mathematical basis of a fluids flow. RANS equations are time-averaged expressions for the motion of a fluid and are essentially derived through Reynolds decomposition where an instantaneous value is broken into its fluctuating and time-averaged components. The atmospheric equations for continuity, motion, and thermodynamic energy express the conservation of mass, momentum, and heat in a volume of fluid. However, the set of RANS equations consists of one or more extra unknown values compared to the number of equations, thereby not permitting a solution to exist for the highly non-linear system of equations in a turbulent flow (Arya 2001). This situation is regarded as the "fundamental problem of closure" and is one of the most

challenging issues faced in simulating turbulent flows (Arya 1999). The closure method chosen defines the speed of processing and the amount of detail in the simulation. Different methods of closure for modeling the Reynold's stress terms, such as introducing eddy viscosity, mixing length, or other turbulence "model" laws and concepts have been developed. These methods are beyond the scope of this report and can be referenced in micrometeorology textbooks such as Arya (2001, 1999).

Another CFD modeling technique using the Navier-Stokes equations is direct numerical simulation (DNS), where no turbulence closure models are needed in solving the Navier-Stokes equations. Instead, the spatial and temporal scales of turbulence are resolved using a fine numerical grid to capture all turbulence scales. This method of CFD modeling is extremely computationally intensive, even in low-turbulence environments (Arya 2001).

CFD modeling through LES is a less resource-intensive approach than DNS that parameterizes the smallest scales of a simulation through a Navier-Stokes equation-based filter (Arya 2001). The initial concept for LES modeling was introduced in the early 1970s for weather and boundary layer meteorology modeling (Deardorff 1970). The "low-pass filter" is a time and space-based method that removes small-scale motions and employs a sub-grid scale model parameterization to address the most resource-intensive processes of turbulence. As a result, CFD modeling with LES is a more advanced higher-order approach that more appropriately captures some of the important physics compared to RANS (Castro et al. 2017). Since LES requires less computational power than DNS, LES promises to be an important area of CFD modeling research, especially for urban flows where LES has been shown to provide better results for simulating concentration distributions around obstacles (Tominaga and Stathopolous 2013).

While CFD codes may appear to be a more accurate option for understanding dispersion, they have their own set of challenges and limitations. The models are more likely to be used for research purposes rather than for emergency response or operational use due to longer processing times, computational requirements, and greater user-learning curve. The local area of simulation has also been shown to tend to be somewhat "disconnected" from larger mesoscale phenomena because assumptions about the vertical structure, surface energy fluxes, and wind patterns are parameterized for computational reasons (OFCM 2002). However, CFD modeling offers a realistic and detailed computational approach for detailing the development and dispersion of a plume within the near-source canopy region (Philips et al. 2013). The U.S. Naval Research Laboratory has introduced a hybrid plume dispersion model using LES called CT-Analyst (Boris et al. 2003). The model produces near real-time contaminant transport predictions of CBR agents in complex urban settings, although pathways for the release scenario and several databases, including the wind fields, must be extensively set up and calculated in advance (Leitl et al. 2016).

5.7 Street Network Models

A newer generation of high-resolution urban dispersion models that simulate a network of interconnected street canyons and intersections among rectangular buildings has been introduced by Soulhac (2000) and further developed by Hamlyn et al. (2007) and Belcher et al. (2015). These street network models require only a few basic inputs and somewhat resemble "modified" Gaussian dispersion models (Ben Salem et al. 2015), as complex building structures are simplified and not explicitly defined. SIRANE was the first operational street network dispersion model to simulate line and point sources within the urban canopy (Soulhac et al. 2011). Instead of portraying a large plume over a domain, the model domain is composed of a 3D network of interconnected streets surrounded by simplified cube shaped buildings. The effects of the flow within the streets have their own parameterizations and are decoupled from the overlying PBL above the urban canopy. A Gaussian plume approach above the canopy accounts for the overall atmospheric dispersion throughout the UBL as pollutants are dispersed within the street canyon based on building geometries. The model has been evaluated against field campaign data

within the city of Lyon, France, and shown to perform reasonably well, although some errors existed among spatial and temporal evolution of the source emissions in the simulation (Soulhac et al. 2012). A more recent adaptation of SIRANE is the SIRANERISK dispersion model, which can simulate steady and unsteady releases above and within the street network and has performed well when compared with wind tunnel studies (Soulhac et al. 2016).

Another street network model called the University of Reading Street-Network Model (UoR-SNM) has also been introduced but avoids velocity flow parameterizations that must be calculated externally before the model can be run (Belcher et al. 2015). In a head-to-head comparison among UoR-SNM, SIRANE, CFD models, and QUIC-generated flow fields, Hertwig et al. (2018) found that the relatively simple street network models performed equally as well as or better than Lagrangian models with 3D wind fields, while also saving computational time and cost. The goal was to study urban dispersion on scales of interest for emergency response applications. SIRANE is currently the only operational street-network model since the UoR-SNM, which is still under development. While these models show promise for urban dispersion applications. One of the biggest hurdles is to adapt the urban morphology employed in these models for use in other locations with vastly different characteristics (Hertwig et al. 2018). Most of the idealized testing was done in European cities that often do not resemble the layout of cities in the United States.

5.8 Comparisons, Strengths, and Limitations for Atmospheric Dispersion Models

Figure 7 and Table 1 provide a visual comparison and show strengths and limitations for the different types of dispersion models.

Gaussian Plume Models	Gaussian Puff Models	Lagrangian Dispersion Models	CFD Models
Typical Computat Seconds	ional Times: Minutes	Minutes to Hour	Hours
• Very fast estimates with minimal	• Fast estimates from a sequence of puff emissions	 Track individual particles downwind 	• Detailed and higher resolution simulation
 Limited spatial or temporal	 Time-varying winds Winds are not 	• Building-resolved features and parameterized	 Based on theoretical physics Bequire expert
variability of windSimplified urban effects included	building-resolved and lack spatial variability	windsRequire considerable	knowledge and resources
by parameterizing plume spread		knowledge and training	AND AND A
Parte Concertation Profiles Weil (4.4.) + V H (1.4.4.)		-	
H + Actions and renger H + Actions and renger = with 40 Bit = plane rise	Plume		
_	Puff		

Increased model complexity, accuracy, and computational requirements

Figure 7: Visual comparison of dispersion models that can be applied for homeland security, emergency preparedness, and emergency response. As the models increase in complexity, so do their computational and user requirements. Many have special applications for urban use. Figure adapted from presentation: *National Atmospheric Release Advisory Center's Urban Plume Dispersion Modeling Capability for Radiological Sources* by Gowardhan et al. (2018) with additional modifications.

MODEL TYPE	STRENGTHS	LIMITATIONS
Box Model	 Commonly used as a screening model Fast and simple calculations with minimal input requirements Can account for simple photochemical production and loss Multiple "boxes" can interact with each other 	 Uniform distribution and single value are calculated for the entire domain Poor representation for point sources in the near field Simplest treatment of input (production) and removal (loss) mechanisms and atmospheric conditions
Gaussian Plume Model	 Uses simple and well-tested, peer reviewed empirical formulas that provide results quickly with relative accuracy, but under simplified conditions Provides reasonable representations of average or long-term downwind concentration behavior Consistent with the random nature of atmospheric turbulence Additional terms can be added or removed to modify the Gaussian plume equation Supported for regulatory use Easy to use and implement Core of many current dispersion models used for emergency situations 	 Recommended for applications no greater than 30-50 km from the source Can be calculated only under a single wind observation under limited spatial and temporal ranges Errors in input meteorology strongly impact the result, especially in more complex and low wind situations Best used for simple terrain without large fluctuations in atmospheric stability Misrepresentation of source term could significantly change model result Rudimentary representation of nocturnal boundary layer May lack spatial concentration variability based on obstacles Inherent uncertainty due to stochastic nature of turbulence
Gaussian Puff Model	 Better than Gaussian plume for representation of time varying meteorological effects ("curved" plume) Strength similar to the Gaussian plume model but can predict ensemble-averaged puff concentration as a function of time as wind speed/direction changes. More accurate in low wind speed situations. Frequently used in emergency situations Sometimes coupled to or implemented as preprocessor for another model Best applied to continuous releases over longer sampling period to account for puff travel time 	 Similar limitations to the Gaussian plume model Unable to capture strong changes in wind variations Difficult to predict ground-level impacts based on puff trajectory Parameterized urban and complex topography (no individual buildings seen) May be less accurate than Gaussian plume model when wind observations are not representative for release location

Table 1: Summary of strengths and limitations for different types of atmospheric dispersion models.

MODEL TYPE	STRENGTHS	LIMITATIONS
Lagrangian Particle Model	 Predicts dispersion under time varying meteorological conditions with different stabilities Continuous, short term, and instantaneous releases Particles are tracked on each time step on a random path to allow greater representation of wind characteristics Includes a type of parameterization for complex or urban terrain More flexibility in source release type Some variations are "CFD-like" but run much faster 	 More complicated to run and higher learning curve than simpler models May take a longer time to run depending on domain (<1 hour) so not always applicable to emergency response More detailed meteorology and source term requirements
Eulerian Grid Model	 Concentration values are calculated for each grid cell in the 3D model for greater spatial coverage, detail, and accuracy Includes photochemical reactions Detailed plume interaction from local meteorology and source characteristics 	 Complex to set up and run, precluding use for emergency response Need to interpolate meteorology using reanalysis data or run "online" with the model Mostly reserved for research applications
Higher Order (CFD and LES Models)	 Offers a realistic and detailed computational approach to detail the development and dispersion of a plume within the near-source canopy region One of the best current representations of dispersion around obstacles in complex environments Provides a denser dataset to evaluate field or laboratory studies Flexibility with source type, domain geometry, and mesh sizes 	 Solves time-averaged RANS equations and users must often outweigh tradeoffs between closure methodologies (i.e., DNS vs. LES) Computationally intensive and usually reserved for research-grade applications rather than operational use Domain of simulation tends to be somewhat "disconnected" from the larger mesoscale systematic behavior
Street Network Model	 A newer generation of high-resolution urban dispersion models that simulate a network of interconnected street canyons and intersections among rectangular buildings Requires only a few basic input conditions Performs equally as well as or better than Lagrangian dispersion models while saving on computational time 	 Research grade – considerable future testing and modification are required to make the models operational. Simplified building geometries that must be adapted to the urban morphology in other locations Most testing has been done in European cities that may not resemble cities of the United States.

6.0 Model Review Process

The remaining sections of this report address Objectives 7 and 8 to document and summarize currently known atmospheric dispersion models into a concise reference table (Section 7.0). Then, a selection of those models is screened for a more in-depth description, intended to serve as a quick reference guide for federal, state, and local agencies and stakeholders requiring dispersion model guidance for emergency preparation or response. The current section briefly describes the model review process, ready-reference table, and methods for choosing a subset of models as part of a two- or three-page reference guide in Section 8.0.

6.1 Quick Reference Table

Ninety-six dispersion models that simulate the fate, transport, and diffusion from an effluent source have been identified in this report. The quick reference table includes dispersion models that can be used for a wide variety of applications, including air pollution dispersion, particles dispersed within the wind flow fields, as well as release agents specific to homeland security threats. Some models are designed for more specific CBRNe applications involving gas, biological particles, and nuclear and explosive dispersion. The purpose of this reference guide is not to recommend or endorse a specific model but to provide users with a resource that documents the currently available models so that the user can make informed decisions. Attempts have been made to keep the information concise and applicable to emergency response officials. While this is a reasonably comprehensive list and assessment of current dispersion models, it is not a completely exhaustive compilation of every known dispersion model both past and present.

The starting point for this list was the early reports from NOAA and US DOE summarizing consequence assessment models (OFCM 1999; Mazzola et al. 1995). These documents were used as the foundation of this work and are described in greater detail in **Section 2.3**. However, many of the models on these lists have not been updated recently, are no longer supported and are obsolete, are specific to certain facility sites (such as particular nuclear power plants or national laboratories), absorbed into newer model formulations, or even included as modules in more powerful and modernized models. One example of this is SCIPUFF, which drives HPAC. In addition, the 3D meteorological fields generated from CALPUFF can also drive MM5, WRF, CTDMPLUS, or ISCST3. Screening-level dispersion models are also not included in this list, but the non-screening version of the model is described. For example, SCREEN3 is the screening model for ISC3.

Literature reviews of peer-reviewed journals, technical reports, internet searches, and discussions with emergency response personnel also led to the current dispersion model list. Models documented in OFCM (1999) that could not be found with a relatively in-depth internet search were not included in the model review and reference table. The internet search included model documentation or mention of the model in any report or journal article. For example, limited information about the outdated "ARCHIE" model is available on the internet search cannot easily find information about a particular model, an emergency response official may use something else. Emphasis has been placed on documenting dispersion models developed or used within the United States, although some well-known and flexible international models are featured in this document.

Section 7.0 provides a quick reference table for obtaining model summaries and other key information. The list is numbered and sorted alphabetically by model name. The second column provides the model name in its expanded and abbreviated form. The best reference source for the model is hyperlinked on the model's short name or abbreviation. This link is likely to be a website with currently

available information, a user's manual, or a description from the developer. For those models, a link is provided to the next best source such as a journal article or other reference document, since some models lack a good source of information online. For printed versions of this report, access to the hyperlinks is available through the digital version. (Note: Some word processors may have trouble opening links to PDF files. To access these websites and documents that are PDFs, copy and paste the link into your internet browser or convert this document to a PDF and then try accessing the link.) The model developer is then provided in the third column. Immediately after this, a one-sentence description outlines the model's core function and purpose. The group of columns 5-10 consists of check boxes to identify the model type (e.g., Gaussian Plume, Puff, Lagrangian, Eulerian, or CFD). Columns 11-14 provide check boxes for the model's intended CBRNe application or the best possible use scenario. There is some flexibility in the identification of *chemical*, as general air pollution dispersion models technically simulate chemical transport. The 15th column identifies the model's best emergency application aligned with the National Planning Framework: either preparedness (including prevention, protection, and mitigation), response (including recovery), or *both*, and is shaded in orange, purple, or blue, respectively. The five emergency response frameworks are grouped into two to simplify the model's best application pre- or post-event. Some models are better designed for planning or response purposes, and it is important for responders to have this key information. The 16th column objectively defines the model's runtime speed and is therefore directly related to its response classification. The yes (Y) or no (N) identification in columns 17-19 indicates whether the model simulates terrain or building effects and whether the model is proprietary. The latter would be Y if the model is site-specific or does not provide the code to users outside its developing entity.

The two rightmost columns in the quick reference table identify if the model was selected for additional review later in this document. A three-tier classification system was applied to the model list where the model was either: 1) excluded from the detailed list (pink), 2) possibly of use for emergency preparation and response, but excluded from the detailed review (yellow), and 3) included in the detailed review (green). If the model was not selected, a brief reason is provided in the final column for yellow and pink classifications. An explanation of this process and number of identified models is outlined in **Table 2**.

6.2 Expanded Model Description

Out of the 96 dispersion models, 40 show viable use for emergency preparation and response purposes, but only 16 were selected for expanded model descriptions. Of those 16 models, four were identified to be best used for emergency planning purposes, and only one was best suited solely for response. Twelve could be applied to pre- or post-release timeframes. The 16 models most viable for emergency preparation, response, or both are expanded in a two- or three-page reference guide which includes the information outlined in **Table 3**.

The information used for each model review was derived from several sources: 1) description, documentation, manuals, and factsheets listed on the model's official website, 2) literature searches of the model's name including peer-reviewed and gray literature, 3) a review of field, laboratory, and real case studies of model applications obtained from internet searches, and 4) outreach to model developers, other specialist users (including this report's author and research team), and emergency responders. Given the broad range of models considered, direct testing of each model was beyond the scope of this review. Ranking each model by a scoring system was also beyond the scope of this report since each model has widely different capabilities and purposes.

Classification	Color Code	Number of Models	Reasoning
Useful for Emergency Response Applications		16	 Developed specifically for emergency preparation, response or for CBRNe applications Widely used and referenced within literature with significant support base Fast and straightforward for most users Free or minimal cost Operational or research grade Includes some application to urban environments Developed and used for applications within the US
Possibly of Use for Emergency Response Applications		24	 Simulates dispersion for some CBRNe applications with some emergency response use Use dependent on need or user's situation Too specific for generic use Not as easy or intuitive for use by non-modelers Moderate to slow running Significant self-research required Mainly research and/or development grade Incorporated within other dispersion models Developed or primarily used for international applications
Not Useful		56	 Not applicable to emergency preparation or response use Site-specific for certain facilities (i.e., specific nuclear power plants or national laboratories) Not widely used or discontinued Difficult or impossible to find information or references Not recently updated or replaced by more advanced model(s) Too expensive, proprietary, or not open source

Table 2: Model classification criteria for inclusion or omission in detailed model review.

Model Criterion	Explanation
Model name and Abbreviation	Short and expanded model name
Developer	Name of company, agency, or individual who developed the model
Type of Model	If the model is built upon a Gaussian Plume, Puff, Lagrangian, Eulerian Grid, or CFD framework
Response Phase	Whether the model is best applied to emergency preparedness, response, or both
Original Application	Whether the model is meant mainly for urban, rural, or complex terrain or has capabilities to simulate around buildings; additionally, the type of CBRNe release(s) the model is best applied for
Model Description	1-2 paragraph description of the model framework, purpose, capabilities, and recent studies, if available
Pros and Cons	Known model advantages, benefits, disadvantages, or shortcomings
Runtime	A general qualitative speed in setting up, running, and post-processing the model results
Input Data Requirements	Typical information or data the user needs to initialize the model and difficulty of preparing these datasets from publicly available information
Outputs	Nature and format of outputs
Data assembly requirements during or after emergency response	As above, but specifically considering the potential of rapidly setting up a model to respond to an emergency
Code language	If known, the computing code foundation the model is developed on for potential debugging
Public or Proprietary, Cost	Model availability and price for government officials, researchers, or individuals
Ease of use	Qualitative measurement of simplicity for responders or researchers, including any barriers to the widespread use in terms of training or specialized hardware or software requirements
Ease of obtaining information and availability of technical support	Ability to request external help, including a user support group, website help pages, or technical support contacts
Source code availability	If the source code is available for dissemination for modification or debugging, if needed
Installation requirements/ software	Hardware computing requirements or specialized technology needed
Maintenance Status	If the model is available for use, undergoing continuous development and improvement, complete, or obsolete, including current version
Documentation	If information on model use and formation is documented in a user's guide or website
Link to Website	Hyperlink to the best-known source of the model, as of Summer 2020

Table 3: Model criteria and explanation of information provided in the expanded model descriptions.

7.0 Dispersion Models– Quick Reference Table

					N	lodel '	Тур	e		CE	3RN	e T	ype							ed
#	Model Full Name and Link to Best Source	Developer	Description	Gaussian Plume	Gaussian Puff	Lagrangian Stochastic Particle	Eulerian Grid	CFD	Other	Chemical	Biological	Radiological/Nuclear	Explosive	Emergency Response Stage	Speed	Terrain Effects?	Building Effects?	Proprietary?	Classification Criteria	Reasons for not including in detail review
1	2DPUF	Westinghouse Savannah River Company	Two-dimensional (2D) modeling system for use alongside Area Evac and the Weather Information and Display System (WINDS) graphical user interface (GUI) for radiological releases under flat terrain at the Savannah River Site (SRS) power plant region		x			-	-			x		Response	Fast	N	N	Y		Not updated since 90s and site-specific
2	ADAM Air Force Dispersion Assessment Model	TMS, Inc. contractor to U.S. Air Force	Modified box and Gaussian dispersion model incorporating effects of thermodynamics, chemistry, heat transfer, aerosol loading, vapor, and dense gas scenarios	x					x	x				Both	Fast (< 5 mins)	N	N	N		Not updated since 90s
3	ADAM Tool Accident Damage Analysis Module Tool	Joint Research Centre of the European Commission, Major Accident Hazards Bureau (MAHB)	Consequence assessment tool developed by the European Union used to simulate toxic airborne concentrations and exposures from chemical fires, explosions, and gaseous cloud releases from industrial facilities built on the SLAB dispersion model	x						x			х	Preparedness	Fast	N	N	Y		
4	ADAPT/ LODI Atmospheric Data Assimilation and Parameterization Tool (ADAPT)/ Lagrangian Operational Dispersion Integrator (LODI)	NARAC, LLNL, DOE	3-D, operational IMAAC advection-diffusion model that calculates possible trajectories, concentrations, and deposition of fluid "particles" in a turbulent flow that represent various types of hazardous releases.			x				x	X	x	x	Both	Mod- erate (<1h)	Y	Y	Y		
5	ADMS 5 Atmospheric Dispersion and Dose Assessment Modeling System	Cambridge Environmental Research Consultants (CERC), United Kingdom (UK)	Advanced model to calculate air quality impacts from point, line, volume, or area industrial sources with algorithms for building and topographical effects.	x	X					x				Preparedness	Fast (mins)	Y	Y	N		Used primarily within the UK for air pollution assessments, limited emergency. response, license required

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6	<u>Aeolus</u>	NARAC, LLNL, DOE	Research model to simulate high-resolution flow and dispersion of hazardous material in urban areas and complex terrain environments for emergency planning guidance.					x		х	x	x	X	Preparedness	Mod- erate (<1h)	Y	Y	Y		
7	AERMOD American Meteorological Society (AMS)/ Environmental Protection Agency Regulatory Model	US EPA, AMS	Rapid, steady-state dispersion model for use in various atmospheric stability conditions for the calculation of downwind receptor concentrations from surface and elevated upwind, stationary sources; one of EPA's preferred and recommended models.	x						x				Both	Fast	Y	Y	N		
8	AFTOX Air Force Toxics Model	US Air Force Phillips Laboratory Directorate of Geophysics	Alternative EPA preferred puff/plume model that determines toxic and maximum chemical gas concentrations at specific locations for continuous or instant surface or elevated releases, sometimes coupled with Wind and Diffusion Over Complex Terrain (WADOCT) for complex terrain.	x	x					х				Both	Fast	N	N	N		Not updated in recently; replaced with more compre- hensive models
9	<u>AI-RISK</u>	LANL	Radiological assessment model used to estimate exposure, health effects, and ground level contamination effects from radioactive waste tank explosions	x								x	x	Preparedness	Fast	N	N	Y		Not emergency response; Specific to Hanford Site
10	ALOHA (CAMEO) Computer-Aided Management of Emergency Operations/Areal Locations of Hazardous Atmospheres	U.S. EPA and the NOAA Office of Response and Restoration	Simple hazard modeling component of the CAMEO software suite designed for use by emergency responders to rapidly plan and respond to numerous types of chemical gas clouds, jets, fires, and dense gas releases by determining threat zones	x						x				Both	Fast	N	N	N		
11	APGEMS Air Pollutant Graphical Environmental Monitoring System	Pacific Northwest National Laboratory (PNNL); DOE	Dispersion and dose assessment prediction model for planning, preparedness, and response applications of stack chemicals and radiological effluent that can be run in three different modes depending on nature of release		x					x		x		Both	Fast	Y	N	Y		Mainly used at DOE's Hanford Site

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12	AOPAC Air Quality Package	Atmospheric Environment Service (AES); Environment Canada	Emergency response model for the prediction of hazard zones from accidental puff or plume chemical releases, included from a large chemical database	x	x					x				Response	Fast	N	N	Y		No recent updates, proprietary and no longer supported
13	ARCON96 Atmospheric Relative Concentrations	NRC, PNNL	Constant straight-line Gaussian dispersion model used to calculate nuclear power plant control room concentrations and habitability from accidental releases of radionuclides through air intakes	x								x		Mostly for Preparedness of accidental releases	Fast	N	Y	N		Not an emergency response model, specific to NRC sites
14	AREA EVAC	Westinghouse Savannah River Company	Transport and dispersion code used alongside 2DPUF for the WINDS GUI to predict radionuclide dispersion and best rally area upon accidental release	x								x		Preparedness	Fast	N	N	Y		No recent updates, site specific to SRS
15	ASPEN Assessment System for Population Exposure Nationwide	EPA	Alternative EPA Gaussian dispersion and mapping tool to estimate toxic air pollutants across a wide area of the US based on rate, location of release, and meteorological conditions, and removal processes for calculating exposure by census tract	x						x				Preparedness	Fast	N	N	N		Mainly for air pollution, mostly replaced by ISC3, AERMOD, and other exposure models
16	<u>AXAIRO</u> <u>AXAOTHER XL</u>	Westinghouse Savannah River Company	Dose assessment code used at the SRS to predict hypothetical nearby and short-term downwind radionuclide doses from inhalation, plume, and ground shine. AXAIRQ considers light to moderate winds while AXAOTHER XL simulates high velocity winds and tornadoes for safety-related documentation	x	x							x		Preparedness	Fast	Y	N	Y		Site specific to SRS
17	BLP Buoyant Line and Point Source Model	Environmental Research and Technology, Inc. (ERT)	Alternative EPA model designed to simulate dispersion associated with stationary line and point industrial sources, particularly aluminum reduction plants, with buoyant plume rise and downwash algorithms	X						x				Preparedness	Fast	N	Y	N		Limited applications (i.e., industrial aluminum plants); now in AERMOD
18	BNLGPM Brookhaven National Laboratory Gaussian Plume Model	Brookhaven National Laboratory (BNL)	Site specific dispersion code used to provide real-time projection of downwind doses of radionuclides released from BNL stacks based on local on-site meteorology	x						x				Response	Fast	N	N	Y		Site specific to BNL

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19	B&M Workbook Britter and McQuaid Workbook	- Britter and McQuaid (1988)	A rapid non-computer-based screening method based on a set of nomograms to provide a hazard estimate of dense gas dispersion and downwind, ground-level concentration from continuous or instantaneous releases	x	x					X				Preparedness	Fast	N	N	N		Not an emergency response model; for screening purposes
20	CALINE4 and CAL3QHCR California Line Source Dispersion Model	California Department of Transportation (Caltrans)	Steady state model for calculating pollution concentrations at receptor locations downwind of highway line sources to assess transportation-related air quality impacts. Replaced by AERMOD as one of EPA's preferred and recommended models.	X						X				Preparedness	Fast	N	N	N		Not an emergency response mode; replaced by AERMOD
21	CALPUFF California Puff Model	Originally Sigma Research Corporation (SRC); now Exponent, Inc.	Multiple component, non-steady state Puff model used to simulate buoyant, puff, or continuous-release, long-range transport of pollutants, emission and removal processes, and sometimes used to drive other dispersion models through high resolution meteorology.		x	X				x				Preparedness	Mod- erate.	Y	Y	N		
22	<u>CANARY</u>	Quest Consultants, Inc.	Hazard assessment model used to model vapor dispersion from pressurized, superheated, and refrigerated liquids, pools, jets, fires, and explosions for a database of many well-known chemicals.	x						х			X	Both	Fast	N	N	Y		Requires purchase from consulting company, designed for industry applications
23	CAP88-PC Clean Air Act Assessment Package - 1988	DOE and EPA	A set of programs and packages for estimating the dispersion, dose, and risk from radionuclide emissions from up to six sources at DOE facilities to ensure compliance with the CAA	х								x		Preparedness	Fast	N	N	N		Not an emergency response model
24	CAPARS Computer-Assisted Protective Action Recommendations System	AlphaTRAC (Terrain Responsive Atmospheric Code)	A modernized version of the TRAC Risk Assessment/Hazard Assessment (RA/HA) model used to produce real-time emergency planning and response dispersion, deposition plumes, and associated health impacts for releases within complex terrain at DOE sites		x					x		x		Both	Fast	Y	N	Y		Designed for use at DOE's Rocky Flats facility

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25	CASRAM Chemical Accident Stochastic Risk Assessment Model	ANL	A statistical analysis model that determines the distribution of hypothetical outcomes of affected populations associated with hazardous chemical release materials stored or transported through an area, using local meteorology and Gaussian/dense gas plume relationships for reporting in the ERG.	x						х				Response	Fast	N	N	N		
26	CATS-JACE Consequence Assessment Tool Set/Joint Assessment of Catastrophic Events	DTRA; FEMA	Estimates the consequences of human and natural disasters to the population, infrastructure, and resources using underlying dispersion models within a GUI and outputs results in geographic information system (GIS) formats for real-time response		x					х	Х	x	X	Both	Fast	Y	N	Y		Capability largely encompassed within HPAC and HAZUS suite; JACE only available to U.S. Federal government
27	CT-Analyst Contaminant Transport Analyst	U.S. Naval Research Laboratory	An instantaneous, 3D LES model depiction of CBRN releases within complex urban areas to aid emergency responders in accidental or intentional windborne contaminant transport threats with fine-scale resolution					x		x	X	x	X	Both	Fast (secs.)	Y	Y	N		
28	CTDMPLUS Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations	EPA	Refined elevated point-source, steady state dispersion model for use in various atmospheric stabilities and terrains, especially for receptors on or near 3D terrain features, and one of EPA's preferred and recommended models.	x						х				Preparedness	Fast	Y	N	N		Mostly for complex terrain-related routine air pollution emissions, not emergency response
29	CUDM Canadian Urban Dispersion Model	Environment and Climate Change Canada	Semi-operational, building aware CBRN dispersion modeling system similar to QUIC and LODI with numerous features that simulate complex urban flow and concentrations from toxic releases at multiple scales to be implemented into Canadian Reach Back Services			x		x		x	X	x	x	Both	Mod- erate	Y	Y	Y		Limited online documentation, model still in improvement stages, mainly for Canadian applications

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30	<u>D2-Puff</u>	Innovative Emergency Management, Inc. (IEM)	A puff/plume model originally designed in the late 1980s as the D2PC model to estimate downwind exposure values of toxic chemical releases, especially those stored at U.S. Army arsenals and DOD sites.	x	x					x			x	Both	Fast	N	N	Y		Now integrated within the JEM
31	DEGADIS Dense Gas Dispersion Model	University of Arkansas; EPA	An alternative EPA dense gas dispersion model used to simulate the concentrations of toxic chemical releases, especially for gases or aerosols heavier than the ambient air, and evaporating, upwardly, or zero-momentum releases and jets over flat terrain.	x						x				Both	Fast	N	N	N		
32	DELFIC/ FPTool Defense Land Fallout Interpretive Code/ Fallout Planning Tool	Oak Ridge National Laboratory (ORNL) and Defense Nuclear Agency	A nuclear fallout and cloud rise prediction and consequence assessment software package, built on SCIPUFF dispersion model and integrated within the Fallout Planning Tool, used to predict radiological concentrations, particle sizes, and dose rates resulting from accidental radiological detonations		x							X		Preparedness	Fast	Y	N	Y/ N		One of the top nuclear fallout codes but hard to find information from ORNL
33	DERMA Danish Emergency Response Model of the Atmosphere	Danish Meteorological Institute	An operational emergency response, long- range (20 km to global), 3D dispersion model that incorporates hybrid stochastic (biological) particle-puff diffusion that is integrated within the Accident Reporting and Guidance System (ARGOS), used primarily within Europe.			x				x	x	x		Both	Mod- erate.	Y	N	N		Used primarily within Denmark and Europe
34	DRIFT 3 Dispersion of Releases Involving Flammables or Toxics	UK Health and Safety Executive (HSE)	Light and dense gas integral dispersion model for simulating plumes from accidental instant and continuous surface releases of toxic and flammable substances	x					X	x				Preparedness	Fast	N	N	Y		Paid alternative to DEGADIS from UK developers, but extensively peer reviewed
35	EPICode Emergency Prediction Information Code	Homann Associates; NARAC; LLNL	Software code that rapidly calculates source terms based on material, height, duration, and form, and neutrally buoyant downwind concentrations of chemicals (gas, vapor, or aerosol) released during hazardous industrial and transportation accidents for use in DOE applications	x	x					x	x			Both	Fast	N	N	Y/ N		Only for use in DOE Emergency Management Issues Special Interest Group

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36	ESCAPE Expert System for Consequence Analysis and Preparing for Emergencies	Finnish Meteorological Institute	A simple Finnish internet browser-based dispersion model and consequence analysis tool used to rapidly estimate flammable and hazardous continuous, instantaneous, and ground-level gas and TIC plume releases to inform emergency responders	x	x					x				Both	Fast	N	N	N		Developed for the needs of the Finnish emergency authorities
37	FEM3MP Finite Element Model in 3-Dimensions and Massively Parallelized	NARAC; DOE	A 3D, time-dependent, CFD-RANS, parallel computing model used to investigate the effects of turbulence, airflow, and dispersion of chemical and biological agents released in a complex urban environment under variable winds					x		x	x			Preparedness	Slow	Y	Y	N		NARAC integrated this model within another urban dispersion model (AUDIM, now Aeolus)
38	FLACS FLame ACceleration Simulator	Christian Michelsen Institute (CMI)	A CFD model used primarily within the oil and gas industry to simulate the consequences from fires, explosions, and toxic gas dispersal out of industrial processing facilities					X		x			x	Preparedness	Mod- erate.	N	N	Y		Not an emergency response model, requires costly purchase
39	<u>Fluent</u>	ANSYS, Inc.	Powerful physics-based, research-grade model for a wide range of CFD applications (flow, turbulence, heat transfer) of gases or particles developed for a multitude of engineering uses					x		x				Preparedness	Slow	Y	Y	Y		Not realistically applicable for emergency response
40	FLEXPART Flexible Particle Dispersion Model	Institute of Meteorology and Climatology (BOKU-Met), Austria	A powerful and flexible long-range, Lagrangian dispersion model used to simulate forward or backward trajectories of particles, gases, vapor, or radionuclides from source to receptor (like HYSPLIT) and recently incorporated into research grade weather forecasting models.			x				x	x	x	x	Both	Mod- erate	Y	N	N		Mainly for research purposes, coupled to models like WRF
41	GENII V.2 Generalized Environmental Radiation Dosimetry Software System – Hanford Dosimetry System v.2	PNNL	A GUI package of radiological consequence analysis software containing five independent atmospheric, exposure, and dispersion models to estimate chronic and acute dose and risk from radionuclide releases in atmosphere or water, developed for EPA exposure research	x	x							x		Preparedness	Fast to Mod- erate	N	Y	N		Not really an emergency response model; used to estimate risk and exposure from NRC sites

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42	HASP Hazard Assessment Simulation and Prediction Suite	UK Defence Science and Technology Laboratory (DSTL), <u>Riskaware</u>	Next-generation information management suite of software tools and models to quickly simulate CBRN dispersion in urban and rural areas to permit emergency and military personnel to more effectively respond and contain hazardous releases for marine, cyber, urban, and biological applications.	?						x	X	x	X	Both	Fast (mins)	Y	Y	Y		Viable incident modeling and response platform but proprietary, license needed, and designed for UK/EU
43	<u>HGSYSTEM</u>	Shell Research, Ltd.	An alternative EPA dispersion modeling system of several computer algorithms used to simulate the source term and different types of hazardous chemical and non-ideal gas releases, especially dense gas (originally for UF ₆). Includes HEGADIS model.	x						x				Preparedness	Fast (1-10 mins)	N	N	Ν		Like DEGADIS in many ways; no recent updates; limited emergency. response applications
44	HIGRAD/ FIRETEC High-Resolution Model for Strong Gradient Applications Fire Behavior Model	LANL and United States Department of Agriculture (USDA) Forest Service	Physics-based 3D code to simulate constantly changing interactions between forest fires, wind flows, fuels, and complex topography.					x		x				Preparedness	Slow	Y	N	Y		Research tool only; main application is for forest fires
45	HOTMAC and RAPTAD Higher Order Turbulence Model for Atmospheric Circulation Random Puff Transport and Diffusion	Yamada Science and Art (YSA) Corporation	An alternative EPA-preferred 3D Eulerian weather model coupled with a puff dispersion model to simulate pollutant flow and dispersion throughout complex terrain and simple urban areas		x					x	x			Preparedness	Fast	Y	Y	Y		No recent updates or model support; use phased into Atmosphere to CDF (A2C) Model
46	<u>HotSpot</u>	NARAC; LLNL	Fast running, field-portable dispersion modeling tools developed for emergency response personnel and planners to provide a close-range (< 10 km), conservative estimate of releases from radiological incidents.	x								x		Both	Fast	Y	N	Ν		

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	HPAC		A comprehensive, robust, operational, and research-grade CBRN dispersion modeling system built upon the SCIPUFF model foundation that predicts the affects of																	
47	Hazard Prediction and Assessment Capability	DTRA	hazardous releases for civilian and military populations by integrating high resolution weather data and modifications for dense gas and urban parameterizations (from Urban Dispersion Model [UDM])		Х					х	х	x	X	Both	Mod- erate	Y	Y	Y/ N		
	HYROAD	National	Hybrid roadway puff model that predicts																	Limited to no
48	Hybrid Roadway Intersection Model	Highway Research Program (NCHRP)	PM from vehicle emissions at receptors within 500 meters of roadway intersections.		х					Х				Preparedness	Fast	N	N	N		response application
	HYSPLIT		NOAA's robust dispersion modeling system that calculates forward and backward air parcel trajectories, pollutant transport, chemical transformation, and deposition of																	
49	Hybrid Single-Particle Lagrangian Integrated Trajectory	NOAA Air Resources Laboratory (ARL)	particles, gases, or aerosols that can be run interactively through an internet browser or downloaded to a computer. HYSPLIT uses high-fidelity weather data for local or long- range dispersion (>1000 miles) with applications for emergency response.			х				Х	х	X		Both	Fast (secs)	Y	N	N		
	INPUFF		A simple, single stationary or moving source Gaussian Puff model that calculates																	Not recently
50	Gaussian Integrated Puff Model	EPA	downwind concentrations from deposition and settling at up to 25 receptors from neutrally buoyant gases released from stack or jet sources.		x					х				Preparedness	Fast	N	N	N		replaced by newer models like AERMOD
51	ISC3	EDA	Alternative EPA steady state Gaussian model used to assess pollutant concentrations from a large number of industrial complex emission	v						v				Proparadaaca	Foot	N	v	N		Replaced by AERMOD; not an emergency
51	Industrial Source Complex Model 3	EFA	sources, including deposition and downwash from stacks.	Λ						Λ				riepareuness	rasi	IN	I	IN		response dispersion model

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52	JEM Joint Effects Model	DOD; Aeris, LLC.	A comprehensive, DOD-accredited, web- based, operational dispersion modeling software built upon SCIPUFF used to simulate accidental or intentional CBRN incidents and weapon strikes across the U.S. Military with advanced capacities for complex terrain, TICs, human health indications, and urban environments, encompassing many standalone dispersion model codes		x					x	x	x	x	Both	Fast	Y	Y	Y		
53	JOULES Joint Outdoor-indoor Urban Large-Eddy Simulation	Aeris, LLC and Lawrence Berkeley National Laboratory (LBNL)	An experimental physics-based LES modeling system that produces high-fidelity simulations of urban and indoor contaminant dispersion for use in operational urban emergency response tools such as the HPAC model, where it is slated to identify performance limitations.					x	x	x	x	x	X	Preparedness	Slow (mins to a few hrs)	N	Y	Y		Experimental and currently research grade only
54	KBERT Knowledge-Based- system for Estimating hazards of Radioactive material release Transients	Sandia National Laboratory (SNL)	A risk analysis tool containing a basic dispersion model, based on stability class, used to estimate the risks and doses for in- facility workers and the nearby public exposed to accidental releases from chemical and nuclear facilities	x						x		x		Response	Fast	N	N	N		Mostly for NRC use, less related to emergency responders; not recently updated
55	KDFOC4 "K" Division Defense Nuclear Fallout Code	- LLNL; NARAC	A nuclear fallout module now incorporated within NARAC's assessment capability that calculates the spread of gamma radiation produced during above or below-ground fission-source detonations by calculating time and weather dependent plume rise	x								x	X	Both	Fast	N	N	Y		Not an emergency response dispersion model
56	LAPMOD LAgrangian Particle MODel	- Enviroware, Italy	3D Lagrangian dispersion model used to simulate dispersion and transport of gases, odors, and inert or radioactive particles over complex terrain from local meteorology.			x				x	x	x		Preparedness	Fast	Y	N	N		Mainly research grade with not much emergency response use
57	LPDM Lagrangian Particle Dispersion Model	National Center for Atmospheric Research (NCAR)	A research-grade model most recently combined with NCAR's EUlerian LAGrangian (EULAG) LES model used to simulate realistic turbulent environments and hazardous release scenarios based on traditional Lagrangian particle dispersion.			x				x	x	x	X	Preparedness	Mod- erate	Y	N	Y		Research grade and largely incorporated within NCAR EULAG model

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58	MATHEW/ADPIC Mass-Adjusted Three- Dimensional Wind Field/ Atmospheric Diffusion Particle-in-Cell	Atmospheric Release Advisory Capability (ARAC), LLNL	Operational 3D wind model coupled with a Lagrangian random walk dispersion model to assess the impact of neutrally buoyant, hazardous first order chemical and radiological releases			x				x		x		Both	Fast (mins)	Y	N	Y		Replaced by newer model (LODI) from NARAC
59	MDIFF	NOAA Air Resources Laboratory Field Research Division	Mesoscale emergency response puff model used to calculate the transport and dispersion of airborne material releases near Idaho National Laboratory (INL), informed by local weather Mesonet and an offspring of original MESODIF model		x					x				Response	Fast	N	N	N		Site specific for use at INL, not recently updated
60	MELCOR and MACCS MELCOR Accident Consequence Code System	SNL	MACCS is a comprehensive, straight-line Gaussian plume model package used to simulate the ecosystem and human dose and exposure impacts of severe nuclear power plant accidents, widely used across DOE facilities from MELCOR model output.	x								X		Both	Fast	N	N	N		
61	MIDAS-AT Meteorological Information Dispersion and Assessment System Anti-Terrorism	ABS Consulting; PLG Inc.	An anti-terrorism puff dispersion modeling system capable of simulating potential hazard areas and aftereffects caused by a chemical or biological agent attack inside a building or urban area, including the spread of an agent between floors and rooms of a building and throughout the urban street canyon.		x					x	X	x		Both	Fast	Y	Y			Limited information available, must purchase
62	MSS PMSS (Parallelized) Micro- Swift Spray	Aria Technologies, France and SAIC	A CFD-like 3D dispersion model coupled with ARIA View designed to simulate complex urban and industrial dispersion by generating mass-constant streamlines and gas or particle plumes around obstacles			X				x			x	Both	Mod- erate (min to <1 h)	N	Y	Y		Mostly French and EU applications, requires purchase
63	NAME III Numerical Atmospheric- Dispersion Modeling Environment	UK Met Office	A sophisticated 3D, random walk, short-to- long range dispersion model used in research, operational, and UK emergency response situations that employs flexible 3D meteorological inputs, unlimited sources, and forward/backward simulations, etc.			x				x	x	X		Both	Mod- erate	N	N	N		Mainly used by UK MetOffice but available for external research use with license

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64	OBODM Open Bum/Open Detonation Dispersion Model	U.S. Army, Dugway Proving Ground	Alternative EPA model that predicts downwind transport, dispersion, and air quality impacts using existing plume rise and dispersion algorithms from open burning and detonations of obsolete munitions and uses algorithms from the Real-time Volume Source Model (RTVSM)	x						x			x	Preparedness	Fast	Y	N	N		Limited emergency response applications
65	OCD 5 Offshore and Coastal Dispersion Model	EPA	Line, point, and area source dispersion model to determine the impact of offshore emissions, plume, and air quality near coastal regions, and one of EPA's preferred and recommended models.	x						X				Preparedness	Fast	Y	N	N		Not updated in many years; most features now in AERMOD
66	OMEGA/ADM Operational Multiscale Environment Model with Grid Adaptivity / Atmospheric Dispersion Model	SAIC	OMEGA is an operational multiscale numerical weather prediction model embedded with an atmospheric dispersion model for use at adaptably large (Eulerian) to small (Lagrangian) spatial scales with many types of parameterizations to simulate gas and particle transport			x	X			x	x			Preparedness	Slow	Y	N	Y		Not recently updated/ replaced with newer model; Minimal internet presence
67	One SAFER One SAFER One HazMat Response	SAFER Systems	A suite of real-time, cloud-based emergency modeling software used to monitor, simulate, and mitigate chemical incidents by allowing users to collaborate across platforms. Designed for emergency responders, and in many ways similar to HASP.		x					x				Both	Fast	Y	Y	Y		Viable real- time response platform, but proprietary, requires license and doesn't share methods
68	OSPM Operational Street Pollution Model	National Environmental Research Institute of Denmark, Aarhus University	An advanced Danish plume and box model used to predict air quality (CO, PM, NO _x) inside urban street canyons from traffic emissions from source to receptor by considering building geometry, urban turbulence, and chemical conversions.	x					x	x				Preparedness	Fast	N	Y	N		No CBRNe applications and not an emergency response model
69	PANACHE Atmosphere Pollution and Industrial Risk Analysis	French Ministry and Environmental Agency (ADEME) and Fluidyn/ Transoft	French proprietary suite of 3D finite fluid mechanics modules for industrial, urban, and complex terrain applications of hazardous accidental or continuous releases					X		X				Preparedness	Mod- erate	Y	Y	Y		Requires user to pay consultant from Fluidyn for risk analysis

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#	Model Full Name and Link to Best Source	Developer	Description	Gaussian Plume	Gaussian Puff	Lagrangian Stochastic Particle	Eulerian Grid	CFD	Other	Chemical	Biological	Radiological/Nuclear	Explosive	Emergency Response Stage	Speed	Terrain Effects?	Building Effects?	Proprietary?	Classification Criteria	Reasons for not including in detaild review
70	<u>PAVAN</u>	Battelle; PNNL	Gaussian plume model used to calculate short- term, ground-level, downwind radiological concentrations from accidental, design flaw- related nuclear power plant releases	x								x		Preparedness	Fast	N	N	N		Not an emergency response model
71	PHAST Process Hazard Analysis Software	DNV Software, UK	Process analysis and hazard consequence tool for mainly industrial sites that examines the behavior of an incident from an initial release to far field dispersion of leaks, ruptures, spills, and toxic clouds.	x	x					x				Preparedness	Fast	X	x	Y		Hazard analysis software rather than an emergency response model
72	PLUVUEII Plume Visibility Model	EPA	Alternative EPA dispersion model that calculates the visual range and atmospheric discoloration (opacity) of plumes caused by single SO ₂ or NO combustion emission sources in Class I (wilderness) areas	x						x				Preparedness	Fast	N	N	N		No emergency response application
73	PUFF-PLUME	PNNL	Emergency puff and continuous plume model that predicts chemical pollution and radionuclide transport, wet/dry deposition, exposure pathways from an accidental release.	x	x							x		Response	Fast	N	N	Y		Site specific to Savannah River Site
74	PUMA Puff Model for Atmospheric Dispersion	- Swedish Defence Research Agency (FOI)	A real-time puff model using Lagrangian dispersion trajectories, with neutral and dense gas chemical capabilities, designed for third party integrations such as FOI's "Dispersion Engine" software package		x					x				Preparedness	Fast	N	N	N		Mainly used in EU; still undergoing development and evaluation
75	QUIC Quick Urban Industrial Complex Model	LANL	Relatively fast-response model that computes various CBRNe agent dispersals, including dense gas, particles, jets, and explosions, on the urban building-to-neighborhood scale with the ability to track dispersion and flow fields around buildings and structures.			x				x	x	x	х	Preparedness	Mod- erate/ Fast (secs - hours)	Y	Y	N		
76	<u>RapidAir</u>	Ricardo Energy and Environment, UK	City-scale, Python-based dispersion modeling system using AERMOD coupled with street canyon model equations where model output kernels are passed over roadway emissions sources (NO _x) to simulate urban air quality	x						x				Preparedness	Mod- erate (mins)	Y	Y	N		Mainly for traffic emissions, not an emergency response model

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#	Model Full Name and Link to Best Source	Developer	Description	Gaussian Plume	Gaussian Puff	Lagrangian Stochastic Particle	Eulerian Grid	CFD	Other	Chemical	Biological	Radiological/Nuclear	Explosive	Emergency Response Stage	Speed	Terrain Effects?	Building Effects?	Proprietary?	Classification Criteria	Reasons for not including in detail review
77	RASCAL 4.3.3 Radiological Assessment System for Consequence Analysis	U.S. NRC	Consequence assessment tool that uses the RATCHET dispersion model for radiological releases from nuclear facilities and powerplants to determine source terms, transport, dose, potential downwind effects, and whether to evacuate or shelter in place.		x							x		Both	Fast	Y	N	N		Mainly used by the Protective Measures Team of NRC for power plants and storage facilities
78	RIMPUFF Risø Mesoscale Puff Model	Risø National Laboratory (Denmark)	An advanced, extensively tested, near real- time mesoscale (<100 km) emergency response model used primarily within Europe to predict the transport and dispersion of CBRN materials and is also incorporated within European emergency centers and response systems (i.e., ARGOS).		x					x	X	x	x	Both	Fast	Y	Y	N		Operationally incorporated in decision support systems but primarily within Europe
79	RLINE Research Line-source Dispersion Model	EPA	A research-grade, line-source dispersion model used to evaluate chemically inert air quality impacts in the near-road environment from mobile sources along and nearby to major roadways using AERMOD's meteorology preprocessor.	x						x				Preparedness	Fast	N	N	N		For traffic related emissions, not an emergency response model
80	Radiological Safety Analysis Computer Program	INL	Modified-Gaussian plume program that calculates the dose, inhalation, ingestion, and air immersion consequences from upwind atmospheric radionuclide releases at nuclear powerplant facilities from accidental or sabotage scenarios on a personal computer	x							X			Both	Mod- erate	N	Y	N		Mainly for use at INL but can be applied to exposure of fission products elsewhere
81	RTDM3.2 Rough Terrain Diffusion Model	ERT	A Gaussian model to estimate ground-level concentrations of chemically stable pollutants and buoyant plume behavior in areas of rough or flat terrain in the nearby vicinity of one or more collocated point sources.	x						x				Preparedness	Fast	Y	N	N		Not updated since 80s; limited CBRNe application

					N	Aodel	Тур	e		CI	BRN	e T	ype							ed
#	Model Full Name and Link to Best Source	Developer	Description	Gaussian Plume	Gaussian Puff	Lagrangian Stochastic Particle	Eulerian Grid	CFD	Other	Chemical	Biological	Radiological/Nuclear	Explosive	Emergency Response Stage	Speed	Terrain Effects?	Building Effects?	Proprietary?	Classification Criteria	Reasons for not including in detail review
82	SCIPUFF SCICHEM Second-order Closure Integrated Puff Model SCIPUFF with chemistry	Titan Corporation; Sage Management (Xator Corp.) Electric Power Research Institute (EPRI)	An alternative EPA second-order closure puff diffusion model used to simulate sequences of 3D, time-dependent puffs from a wide variety of source geometries and types with flexible meteorology inputs. The chemistry version models the transport, dispersion, and chemical reactions of gases and aerosol releases from single or multiple sources. SCIPUFF is the transport and dispersion code of HPAC, JEM, and is also integrated with other models.		x					x				Both	Mod- erate	Y	Y	Ν		See HPAC or JEM entry
83	SDM Shoreline Dispersion Model	EPA	An alternative EPA model used to determine ground level concentration from tall stationary point sources influenced by meteorological phenomena near shoreline environments affecting plume behavior and fumigation.	x						X				Preparedness	Fast	Y	N	N		Not emergency response related
84	SHARC/ERAD Specialized Hazard Assessment Response Capability/Explosive Release Atmospheric Dispersion	SNL	A suite of five models (Nuke, AIRRAD, Blast, and ERAD/PUFF, MCK) that simulates the release of radioactivity from nuclear weapon explosions or detonations. The Gaussian puff model, ERAD, is used to predict the radiological detonation dispersion and to assess time dependent, dynamic explosive buoyant plume rise for exposure and evacuation criteria.		x							x	X	Both	Fast	N	N	Ν		
85	<u>SIRANE</u>	Atmosphere, Impact & Risk (AIR), Ecole Centrale de Lyon, France	The first and currently only fine-scale street- network dispersion model designed to simulate the flow and dispersion through a network of interconnected streets with a Gaussian approach to the adjacent urban boundary layer above the street canopy.	x					x	X				Preparedness	Fast	N	Y	N		Currently in development stages; mainly for European city geometries
86	<u>SLAB</u>	LLNL	Alternative EPA dense gas model also incorporated in ALOHA and ADAM Tool to simulate jet, volume, evaporating pool, and volume continuous or instant releases from accidental or intentional episodes.	x	x					x				Both	Fast (mins)	N	N	Ν		See ALOHA or ADAM Tool entries

					N	Iodel	Тур	e		CB	RN	e T	ype							ed
#	Model Full Name and Link to Best Source	Developer	Description	Gaussian Plume	Gaussian Puff	Lagrangian Stochastic Particle	Eulerian Grid	CFD	Other	Chemical	Biological	Radiological/Nuclear	Explosive	Emergency Response Stage	Speed	Terrain Effects?	Building Effects?	Proprietary?	Classification Criteria	Reasons for not including in detail review
87	STILT Stochastic Time-Inverted Lagrangian Transport Model	Harvard University, MPI-Jena, University of Waterloo, and Atmospheric & Environmental Research (AER)	A research-grade, Lagrangian particle dispersion model used to derive upwind source region concentrations and fluxes, such as greenhouse and trace gas releases, based on fixed downstream measurement receptors and driven by high resolution weather prediction models			х				x				Preparedness	Fast	Y	N	N		Generally for air pollution applications; not an emergency response model
88	TAPM The Air Pollution Model	Commonwealth Scientific and Industrial Research Organisation (CISRO), Australia	An advanced 3D model coupled with a weather and Lagrangian particle model to simulate the dispersion of emissions sources in local-to-urban areas, including plume rise, building wakes, and atmospheric chemistry.			х	x			X				Preparedness	Mod- erate	Y	Y	N		For air pollution; not an emergency response model
89	TRACE Toxic Release Analysis of Chemical Emissions	SAFER Systems	Consequence assessment chemical mass- balance tool to simulate and visualize airborne hazard material releases from chemical incidents, including sprays and dense gas, to update risk assessments and EPA RMP plans at chemical sites.						x	X			x	Preparedness	Fast	N	N	Y		Risk assessment; not an emergency response model; See One Model
90	UDM Urban Dispersion Model	UK DSTL	The urban-based model currently incorporated within HPAC that modifies a plume based on street alignment and building density in urban areas but does not resolve dispersion around individual buildings.		x					x	X			Preparedness	Mod- erate	Y	Y			See HPAC entry
91	UoR-SNM University of Reading Street Network Model	University of Reading, UK	A research-grade, street network urban dispersion model similar to the operational SIRANE model, but without flow parameters, that represents particle flow within an urban area as a system of connected boxes at intersections.						x	X				Preparedness	Slow	N	Y	Y		Requires LES flow fields; research grade so not realistic for emergency response
92	<u>VALLEY</u>	EPA	An EPA alternative steady-state screening tool for rural and complex terrain to estimate 24-h average pollutant concentrations for point or area sources (stacks or industrial areas), related to predecessor VALDRIFT model.	x						x				Preparedness	Fast	Y	N	N		Screening dispersion model only
93	VAPO Vulnerability Analysis and Protection Option	DOD, DTRA, Applied Research Associates (ARA)	A 3D vulnerability and risk assessment software tool (rather than a dispersion model) that predicts effects of structural damage, injury, and human risk from terrorist related CBRNe blasts at building sites in urban areas.						X				x	Both	Fast (mins)	Y	Y	Y		Assesses risk and structural impacts from a blast rather than dispersion

					N	Iodel	Tyj	pe		Cl	BRN	le T	ype							ed
#	Model Full Name and Link to Best Source	Developer	Description	Gaussian Plume	Gaussian Puff	Lagrangian Stochastic Particle	Eulerian Grid	CFD	Other	Chemical	Biological	Radiological/Nuclear	Explosive	Emergency Response Stage	Speed	Terrain Effects?	Building Effects ?	Proprietary?	Classification Criteria	Reasons for not including in detail review
94	VENTSAR XL	Westinghouse Savannah River Company	An Excel-based Gaussian dispersion model that incorporates plume rise and building effects, used to determine downwind doses and risk from exhaust effluent.	x						x		x		Preparedness	Fast	N	Y	Y		Not recently updated; not emergency response; designed for
95	VLSTRACK Vapor, Liquid, and Solid Tracking	U.S. Naval Surface Warfare Center	Hazard prediction model used by DOD to provide downwind hazard predictions for a range of chemical and biological warfare agent attacks, including munitions.		x					x	x			Preparedness	Mod- erate	N	N	Y		Incorporated within JEM model
96	<u>XOQDOQ</u>	PNNL	Gaussian dispersion model used to calculate long-term, routine, intermittent, or expected release concentrations and depositions at radial distances up to 50 miles out from nuclear reactor site.	x								x		Preparedness	Fast	N	N	N		Not an emergency response model, retired
8.0 Expanded Model Descriptions

8.1 ADAM Tool

Accident Damage Analysis Module (ADAM) Tool

Developer	Joint Research Centre (JRC) of the European Commission (EC), Major Accident Hazards Bureau (MAHB)
Type of Model	Gaussian Puff and Plume Dispersion Model
Response Stage	Emergency Preparedness
Original Application	Chemical and explosive releases from hazardous industrial accidents
	The ADAM Tool is a software package developed by the EU's JRC to assess the consequences and damages associated with an accidental, hazardous industrial chemical release. ADAM is designed to be a comprehensive consequence assessment tool to simulate toxic airborne concentrations and exposures from chemical fires, explosions, and gaseous cloud releases from industrial facilities for prevention and preparedness. The model can support industrial risk management, land use and emergency planning, enforcement of regulations, inspection and monitoring, and identify weak areas for site improvement (Fabbri and Wood 2019). It contains an extensive database of substances, their physical properties, and exposure effects (i.e., LD50 and IDLH). The ADAM Tool can calculate the physical hazard situations and human health impacts that may arise from thermal radiation, over- pressurization of tanks, flammable releases, explosions, and loss of containment of a toxic chemical. The model contains a GIS mapping tool to assess spatial risk of the affected area.
Model Description	ADAM contains three modules that track the dangerous substance from loss of containment to impact on affected populations. The first module requires the source term, including the amount released, flow rate, and thermodynamic state of the released agent. The second module estimates the physical effects from the release (i.e., fires, explosions, toxic clouds) and its local dispersion. The vulnerability is calculated in the third module to inform the potential level of harm to exposed individuals based on intensity, dose, and exposed duration for the specific release to initiate protective action and lifesaving measures. The dispersion modeling component is built upon the existing and well verified SLAB Gaussian Puff/Plume model developed by LLNL. SLAB is commonly applied to dense gas scenarios, although it can simulate neutrally buoyant and lighter than air releases. ADAM can model continuous, finite, and instantaneous releases from source types including ground-level evaporating pools (area releases), horizontal or vertical jets, and stacks or elevated releases. All effluent can be gases, aerosols, or a combination of liquids and gases. The SLAB code was rewritten and streamlined into the ADAM Tool. A comprehensive model evaluation was performed by Fabbri and Wood (2019) by conducting a series of relevant release scenarios and benchmarking the results with similar software and experimental field datasets. The ADAM Tool was found to simulate various release scenarios well using the default model

	options. The most recent evaluation has been done with the Jack Rabbit II (JRII) chlorine field study dataset (Fabbri et al. 2020).
Pros	Modern, evaluated modeling tool built upon a well-used dispersion modeling platform; calculates vulnerability and physical health effects
Cons	Does not consider environmental consequences; primarily used for emergency preparation within EU nations; requires detailed information about the release
Runtime	Fast
Input Data Requirements	General knowledge of meteorological conditions; detailed specifics about the release mechanism and agent
Outputs	Dispersion plume of effluent and hazard area contour maps; vulnerability and physical harm regions for exposed individuals; graphs of relevant parameters from the release; lethality curves
Data assembly requirements during or after emergency response	Knowledge of meteorological conditions; release mechanism and agent information
Code language	C++
Public or Proprietary, Cost	The model is primarily an EU tool used to support implementation of the Seveso Directive (control of major hazardous accidents). It is available to EU countries or other regulators associated with chemical safety and security. However, it is also available to Organisation for Economic Co-operation and Development (OECD) countries (the U.S. is an OECD country). Distribution is made on request to interested government users (and some non-commercial research users) that fit these criteria. It is not available to consultants.
Ease of use	Not known
Ease of obtaining information and availability of technical support	General queries can be sent to: <u>JRC-MINERVA-Info@ec.europa.eu</u>
Source code availability	No
Installation requirements/ software	Not known
Maintenance Status	The model was launched in 2019 and is available to interested counties and government organizations (Fabbri and Wood 2019)
Documentation	The technical guidance document is available at: https://publications.jrc.ec.europa.eu/repository/bitstream/JRC107633/kjna2873 2enn.pdf
Link to Website	https://adam.jrc.ec.europa.eu/en/adam/content

8.2 ADAPT/LODI

<u>Atmospheric Data Assimilation and Parameterization Tool (ADAPT)/ Lagrangian</u> <u>Operational Dispersion Integrator (LODI)</u>

Developer	National Atmospheric Release Advisory Center (NARAC), Lawrence Livermore National Laboratory (LLNL), DOE
Type of Model	Lagrangian Particle Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Various CBRNe releases for operational use throughout urban or rural areas
Model Description	ADAPT/LODI is a 3-D, Lagrangian, operational transport and diffusion model that calculates possible trajectories, concentrations, and depositions of fluid "particles" in a turbulent flow. The particles are intended to represent various types of hazardous CBRNe releases, ranging from thermal or momentum driven releases from stacks or fires, to detonations from chemical explosives or nuclear sources. The model is NARAC's chief operational emergency response resource for IMAAC's plume generation service. The system contains two models: 1) ADAPT, which is used to construct 3D meteorology fields for use in 2) LODI, the Lagrangian dispersion model. ADAPT develops key meteorological parameters including winds, temperature, pressure, humidity, and precipitation. These variables are obtained from the most recent NWS observations (such as airport sites, weather balloons, and weather networks) when results are needed instantaneously. For extended or ongoing atmospheric releases, gridded model datasets or other weather models, such as WRF, may be used (Nasstrom et al. 2007). ADAPT creates wind fields using the finite element method (a method of solving equations over a large area divided into smaller and simpler parts), which is also beneficial over nonhomogeneous and complex terrain. ADAPT can produce input for LODI within one minute (Bradley 2005).
	The LODI model employs a Lagrangian stochastic Monte Carlo approach (which calculates an average based on a nearly Gaussian distribution of atmospheric turbulence) and then solves the 3D advection-diffusion equations. The model can produce a time series of instantaneous and time-integrated effluent concentrations and depositions, as well as a detailed plume within 5-15 minutes. The model can simulate dispersion for a variety of spatial and temporal scales, including dispersion over regional to local scales. LODI can integrate multiple point, line, area, spherical, or moving sources, including variable emissions rates. Particle size distributions, radiological decay, wet and dry deposition, and resuspension algorithms are also incorporated within the model. Results can be output to GIS mapping tools where spatial analyses can inform responders of protective action zones, exposure guidelines, and regions where doses exceed safe levels. ADAPT/LODI has evolved from the MATHEW-ADPIC and ARAC ² models since the 1990s.

² See information about ARAC at: <u>https://narac.llnl.gov/content/mods/publications/op-model-description-evaluation/UCRL-JC-125034.pdf</u>

Pros	Produces results rapidly; proven to be an effective operational model;
Cons	Not fine scale enough to predict dispersion at the street or neighborhood level within urban areas
Runtime	Generally fast, within 5-15 minutes depending on the domain
Input Data Requirements	Location of the release and source characteristics
Outputs	Processed outputs result in maps of air or ground contamination, dose, and health effects resulting from the release, including protective action zones
Data assembly requirements during or after emergency response	Location of the release, local meteorology, and source characteristics
Code language	Unknown
Public or Proprietary, Cost	Proprietary, but use may be granted for some research and development applications
Ease of use	Moderate
Ease of obtaining information and availability of technical support	Questions can be directed to <u>owner-narac-web-spt@listserv.llnl.gov</u> who will forward the request to the appropriate individual
Source code availability	No
Installation requirements/ software	Unknown
Maintenance Status	Currently used as an operational model within NARAC for IMAAC
Documentation	
Link to Website	https://narac.llnl.gov/tools/operational-modeling/dispersion-model-lodi

8.3 Aeolus

<u>Aeolus</u>

Developer	NARAC (National Atmospheric Release Advisory Center), Lawrence Livermore National Laboratory (LLNL); DOE
Type of Model	Computation Fluid Dynamics (CFD) Model
Response Stage	Emergency Preparedness
Original Application	CBRNe CFD model for complex terrain and urban research applications
ApplicationCBRNe CFD mAeolus is NAR high resolution and complex tel emergency plar code based on to volume surrour within NARAC 	Aeolus is NARAC's primary research and development model that simulates high resolution flow and dispersion of hazardous material through urban areas and complex terrain environments. The model, which is generally used for emergency planning guidance, is a physics-based and building-resolving CFD code based on the finite volume method (solving equations on the small volume surrounding a point on the computational mesh/grid). Aeolus is used within NARAC's operational emergency response applications alongside ADAPT/LODI, but mainly for emergency planning guidance. Even though Aeolus is still a research-grade model, it is being phased into operational use for the generation of urban products for state and local agencies though IMAAC (Gowardhan et al. 2018). The model can simulate releases from nuclear power plant accidents, detonations, toxic industrial chemical spills, RDDs, and biological and chemical agents. Aeolus can be run under a fast, operational mode using a RANS solver for potential operational use or when many simulations are needed. Alternatively, it can be run at high resolution through the more detailed LES method for research and planning. The operational mode can produce results within 5-10 minutes on a laptop, but the LES simulation takes several hours. As with other RANS models, Aeolus solves the incompressible Navier-Stokes equations on a staggered Cartesian grid. Aeolus RANS consists of a solver to produce the steady state wind and turbulence fields as well as a Lagrangian dispersion model to predict the contaminant dispersion throughout the urban morphology. Radiological source terms and half-life behaviors have also been integrated into Aeolus based on explosive plume rise. The model can also simulate buoyant and dense gases and particles. To facilitate faster model setup times in
	urban areas, building profile domains have been generated and stored within NARAC's geographical database for over 130 cities across the US. Terrain data are also available on a 10 m grid across the US. Meteorology can be input through forecast model data (i.e., HRRR, NAM, GFS), or through a wind profile specified by the user. Aeolus has evolved from the FEM3MP model to AUDIM over the past several years. It has been extensively evaluated against the Joint Urban 2003 field study and shown to produce good agreement (Lucas et al. 2016).
Pros	RANS model generally has fast runtimes; resolves building profiles for urban dispersion; Evaluated against field data and showed good agreement

Cons	Highest resolution simulation could take hours; mainly for research and development purposes
Runtime	Variable depending on simulation choice; RANS simulation about 5-10 minutes, high resolution LES takes several hours on laptop
Input Data Requirements	Latitude and longitude of the release, domain size, resolution, period of simulation, and details about the source, meteorology
Outputs	Time evolving spatial plots (exportable to GIS mapping software) of the dispersion of particles downwind of release; 3D deposition on surfaces, effective dose and hazard zones near release
Data assembly requirements during or after emergency response	Location of the release, source characteristics, and meteorology (expected to take only about 2 minutes)
Code language	Unknown
Public or Proprietary, Cost	Proprietary, but use may be granted for some research and development applications
Ease of use	Moderate
Ease of obtaining information and availability of technical support	Questions can be directed to <u>owner-narac-web-spt@listserv.llnl.gov</u> who will forward the request to the appropriate individual
Source code availability	No
Installation requirements/ software	Unknown
Maintenance Status	Currently being used and developed by NARAC
Documentation	See website for more information
Link to Website	https://narac.llnl.gov/research-and-development/urban-dispersion-modeling

8.4 AERMOD

<u>American Meteorological Society/Environmental Protection Agency Regulatory</u> <u>Model (AERMOD)</u>

	U.S. EDA and American Metaonological Society (AMS), Developed by
Developer	AERMIC (American Meteorological Society/EPA Regulatory Model Improvement Committee)
Type of Model	Gaussian Plume Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Gaussian plume model to determine regulatory, source permitting, and downwind concentrations from source to receptor in steady state conditions
Model Description	AERMOD is EPA's preferred and recommended Gaussian dispersion model to simulate the concentration of gases and particles at downwind receptors from surface and elevated stationary sources (Cimorelli et al. 2005). It is a steady-state model for use in various atmospheric stability conditions based on the PBL structure. The model incorporates a well-established boundary layer, scaling, and turbulence concepts and parameterizations. Under stable atmospheres and low turbulence conditions, the model applies a Gaussian approach. During unstable, convective periods, it uses a non-Gaussian method for the vertical component of the plume. AERMOD includes special treatment for single or multiple point, area, and volume sources. It accounts for plume rise, the effects of building downwash, complex terrain for point sources, limited interactions within urban areas, and wet and dry deposition. The model produces concentrations for an array of downwind receptors. The user can specify the quantity and density of the receptor sites for the most appropriate dispersion representation. AERMOD is EPA's primary regulatory dispersion model to assess concentration fields at emission sites. It is specifically used for New Source Review (to issue emission source permits, such as at industrial locations), to develop State Implementation Plans, formulate mitigation plans for non-attainment areas using NAAQS, and to generally evaluate the effects and behavior of downwind effluent dispersion. AERMOD simulations are set up with the use of two data input preprocessors. AERMET is the meteorological preprocessor that defines the meteorological state of the PBL. AERMAP is a terrain data preprocessor that implements U.S. Geological Survey (USGS) Digital Elevation Data and has algorithms that determine the terrain features used by AERMOD. Other preprocessors may optionally be used. AERSCREEN can rapidly run the AERMOD and BPIPPRM incorporates multiple building dimensions near the source to provide an effective building for building downwash calcul

	evaluated through field tests. AERMOD has replaced or incorporated many older models such as BLP and OCD5. It was originally promulgated as a replacement to ISCST3 ³ .
Pros	Fast runtimes; widely supported by EPA as the preferred regulatory model for source permitting, SIP analysis, and traffic conformity studies; free; theoretical concepts supported by field and laboratory studies
Cons	Susceptible to all limitations of Gaussian plume models; may underpredict concentrations in some situations; model setup may be somewhat challenging for some users; limited to downwind receptor distances of about 20-50 km; does not account for different types of CBRNe releases
Runtime	Fast; within seconds, but depends on number of sources, receptors, and simulation periods
Input Data Requirements	Meteorological state of the PBL (e.g. wind, temperature, stability), surface and terrain characteristics, source location and release characterization, location of the downwind receptors
Outputs	Concentrations at downwind receptors
Data assembly requirements during or after emergency response	Local wind speed and direction near the source to construct a vertical wind profile, effluent source characteristics
Code language	FORTRAN
Public or Proprietary, Cost	Free through EPA's SCRAM website; companies such as Lakes Environmental (<u>https://www.weblakes.com/products/aermod/index.html</u>), Breeze Software, and Enviroware offer AERMOD within more user-friendly GUI windows, but the cost is not insignificant (over \$1,600 for AERMOD View by Lakes). Some companies offer free accounts for EPA or government employees
Ease of use	Moderate, runs from a Windows command line prompt. The model is easier to run if used through paid GUIs
Ease of obtaining information and availability of technical support	Support for the EPA SCRAM website can be obtained by contacting George Bridgers: <u>bridgers.george@epa.gov</u> . The SCRAM website posts a wide range of support documents, test cases, and evaluation reports. Many companies also provide consulting services
Source code availability	Yes, available on EPA's SCRAM website along with executables
Installation requirements/ software	32- or 64-bit Windows PC

³ See: <u>https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models#aermod</u>

Maintenance Status	Continuously updated and improved by EPA, most recent version as of mid-2020 is AERMOD v19191
Documentation	A comprehensive user guide is available at: <u>https://www3.epa.gov/ttn/scram/models/aermod/aermod_userguide.pdf</u> . Several quick reference guides are also available on the SCRAM website
Link to Website	https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and- recommended-models#aermod

8.5 ALOHA (CAMEO)

Computer-Aided Management of Emergence	y Operations/Areal Locations of Hazardous
Atmospheres (CAMEO/ALOHA)	

Developer	U.S. EPA and the NOAA Office of Response and Restoration
Type of Model	Gaussian Plume Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Local dispersion and threat zone estimation during accidental chemical releases
Model Description	CAMEO/ALOHA is a simple hazard modeling package designed for emergency responders. The software can help decision-makers rapidly plan and respond to numerous types of chemical gas clouds, jets, fires, and dense gas releases within a range of 100-10,000 meters of the release ⁴ . The software determines threat zones which provide an estimate of downwind distance where proactive measures should be taken. If NOAA or EPA is activated by IMAAC reach back support, CAMEO/ALOHA may be used. The software package contains four distinct entities: 1) CAMEO Chemicals, 2) CAMEO/m, 3) ALOHA, and 4) MARPLOT. CAMEO Chemicals is a comprehensive, proprietary database of hazardous chemical datasheets and chemical physical properties that provides information similar to that in the classic orange US DOT ERG. CAMEO Chemicals rapidly displays descriptive properties of the chemical of interest. CAMEO/ <i>m</i> is a database used to develop planning guidance about chemicals within a local community such as details about a specific facility, chemical transportation routes, and emergency response procedures. The plotting software in CAMEO is MARPLOT.

⁴ For more information, see: <u>https://www.epa.gov/cameo/what-cameo-software-suite</u>

Pros	Simple, easy to use model for first responders; free and widely distributed; comprehensive database of chemicals; fast model result
Cons	Lacks some simple additions like plume rise and certain custom user inputs; susceptible to all limitations of Gaussian plume models; results best used for informative guidelines
Runtime	Fast, seconds
Input Data Requirements	Local atmospheric conditions, identity of the chemical, and details about the spill scenario
Outputs	Threat zone estimates within a grid in ALOHA can be plotted on maps in MARPLOT, GIS software, or Google Earth
Data assembly requirements during or after emergency response	General idea of local weather conditions (wind speed and direction), chemical type released
Code language	C and some Python
Public or Proprietary, Cost	Freely available through EPA's website: <u>https://www.epa.gov/cameo/aloha-software</u>
Ease of use	Easy, software used through the CAMEO GUI
Ease of obtaining information and availability of technical support	Questions, comments, suggestions, and software issues can be addressed by emailing the RMP Reporting Center: <u>RMPRC@epacdx.net</u> , NOAA's Office of Response and Restoration: <u>orr.cameo@noaa.gov</u> , or by calling the CAMEO help desk at (703) 227-7650. Training can be found through: <u>https://response.restoration.noaa.gov/training-and-</u> <u>education/training/workshops/cameo-training.html</u>
Source code availability	Yes, but since the chemical database is a proprietary component, a user license must be set up with the American Institute of Chemical Engineers at the cost of \$3,400 per year through <u>www.aiche.org/dippr</u> . The source code itself is free, but a license is still required.
Installation requirements/ software	Most Windows PC or Mac operating systems, with capability as far back as Windows 7 and iOS Mountain Lion (10.8); portable versions on smartphones are also available
Maintenance Status	Regular updates to the chemical library, user interface, program functionality, and help documentation. Most recent version as of mid-2020 is Version 5.4.7, last updated in September 2016
Documentation	ALOHA Technical Documentation for v5.4.4 is found at: <u>https://response.restoration.noaa.gov/sites/default/files/ALOHA_Tech_Doc.pdf</u>
Link to Website	https://www.epa.gov/cameo/aloha-software and https://response.restoration.noaa.gov/oil-and-chemical-spills/chemical- spills/aloha

8.6 CALPUFF

California Puff Model (CALPUFF)

Developer	Sigma Research Corporation (SRC), now Exponent, Inc.
Type of Model	Lagrangian, Gaussian Puff Dispersion Model
Response Stage	Emergency Preparedness
Original Application	Moderate to long-range transport of gaseous substances through even and complex terrain
Model Description	CALPUFF is a non-steady state Lagrangian Puff model used to simulate buoyant, instantaneous, or continuous-release, long-range transport of airborne contaminants (i.e., PM, SO _X , NO _X , or inert particles) (Scire et al. 2000). As opposed to a steady-state model, CALPUFF can simulate multiple emission and removal processes at various rates by not necessarily maintaining equilibrium. The model is listed as one of EPA's alternative dispersion models for assessing long range transport of pollutants and its impacts on human health and the environment. It has the capability of simulating time-varying point and area sources, domains as small as few hundred meters to a large as hundreds of kilometers, simulation times from one-hour to one-year, chemical conversion and removal mechanisms, and special treatments for complex terrain (Scire et al. 2000). It consists of wet and dry deposition, building downwash, and fumigation algorithms. The model can also account for low wind speeds, near-field impacts from source to receptor, and regulatory air quality applications (such as attainment areas, visibility, and criteria pollutants). CALPUFF includes three main modules that aid in pre- and post-processing.
Model Description	CALMET is a 3D meteorological model to develop hourly wind and temperature fields for the gridded domain. Specifications of the PBL and local topography (including terrain blocking flows or bodies of water) are also included. CALPUFF is the transport and dispersion model that advects puffs of effluent released from emission sources. The model uses the meteorology generated from CALMET to predict the downwind dispersion and puff behavior. Non-gridded, simplified wind profile data may also be used if CALMET is not run. CALPUFF then produces hourly concentration and deposition values at user-specified receptor locations downwind of the release. CALPUFF tracks the puffs using a Lagrangian frame of reference. The final component called CALPOST processes the model output to summarize the results into average and maximum concentrations at the receptors. Additional modules aid in quality control checks and flexibility for reading in meteorological or terrain data. To enhance the functionality, each component of the model can be run through an optional GUI window to prepare, configure, and run the model. CALPUFF also interfaces with other meteorological models such as MM5 and WRF to allow greater support for localized meteorological processes.
Pros	Continuously updated, well-tested, and listed as an EPA alternative dispersion model; permits long run times at distances as great as 200 km downwind of source

Cons	Limited emergency response use, mainly used to perform analyses that help address regulatory and air quality issues; could have a large learning curve
Runtime	Depends on number of sources, receptors, and length of simulation; could be seconds to hours
Input Data Requirements	At a minimum, a wind and temperature profile; source type, emission rate, and locations of receptors
Outputs	Average and maximum concentrations at the user-specified downwind receptors; indication of atmospheric visibility and regulatory air quality attainment at each receptor
Data assembly requirements during or after emergency response	Wind and temperature profiles, emission source specifics
Code language	FORTRAN
Public or Proprietary, Cost	Freely available to anyone through Exponent, Inc.'s website; a more user- friendly version is also available with a streamlined GUI and postprocessing system by Lakes Environmental or Breeze Software: <u>https://www.breeze-</u> <u>software.com/software/calpuff</u> although the price is \$3,595. Private consultants will also run the model for a cost.
Ease of use	Moderate, when used with a GUI window.
Ease of obtaining information and availability of technical support	The GUI windows contain an extensive help system. Training can be obtained from the Exponent developers. EPA provides some reference guides on SCRAM website.
Source code availability	Yes
Installation requirements/ software	Windows PC
Maintenance Status	As of mid-2020, the standard, stable distribution version is CALPUFF v7.2.1. CALPUFF v7.3.1 is also available as a beta release. V5.8.8 is EPA's approved alternative regulatory version of the model.
Documentation	User's guide for CALPUFF v6 can be downloaded at: <u>http://www.src.com/calpuff/download/CALPUFF_Version6_UserInstructions.pd</u> <u>f</u> with an addendum for v7 at: <u>http://www.src.com/calpuff/download/download.htm</u>
Link to Website	http://www.src.com/

8.7 CASRAM

Developer	Argonne National Laboratory (ANL)
Type of Model	Statistical Analysis tool incorporating a Gaussian Plume Dispersion Model
Response Stage	Emergency Response
Original Application	Straight line Gaussian plume model for chemical releases over simplified even terrain
Model Description	CASRAM is a statistical analysis model that determines the distribution of hypothetical outcomes of affected populations associated with hazardous chemical releases of materials stored or transported through an area. Using chemical shipment profiles, routes, and meteorology inputs, the model runs tens of thousands of incidents for rail and highway chemical accidents (Brown et al. 2017). The statistical plume results are then reported in the U.S. DOT's ERG for protective action distances and routing-based risk assessments (Brown et al. 2001). Most recently, CASRAM was run for technical guidance in the 2016 ERG book (Brown et al. 2017) with a forthcoming report for the 2020 ERG. The model predicts hazard zone distributions to identify the threshold chemical concentration where local populations could be affected. It employs a Monte Carlo statistical analysis framework, which sets it apart from other Gaussian models like ALOHA or SCIPUFF. CASRAM determines the distribution of possible outcomes to provide a probability for each specific release consequence. EPA and OSHA health exposure guidelines and associated consequences are also estimated. The model simulates both the physical and thermodynamic-related effects of a hazardous chemical release by computing fixed or time-varying release rates from tanks in liquefied, compressed, evaporated, or flashed chemical states. A dense gas algorithm was added after the 2000 ERG using empirical entrainment parameterizations from the DEGADIS model formulation (Brown et al. 2017). Chemical reactivity, deposition, and various empirical surface types and atmospheric stabilities are also incorporated within the model. A weather and climate database for over 200 cities customizes the statistical analyses based on region and state.
Pros	Theoretical atmospheric dispersion framework built upon existing and sound principles; model results published and updated in each ERG version for practical emergency responder use
Cons	Model is not generally available for use outside ANL but used to inform resources used by responders
Runtime	Fast
Input Data Requirements	Chemical release rate, type, and amount; general meteorological conditions (wind and atmospheric stability)
Outputs	Statistical analysis of hazard zones following accidental container releases

Chemical Accident Statistical Risk Assessment Model (CASRAM)

Data assembly requirements during or after emergency response	Chemical release rate, type, and amount; general meteorological conditions
Code language	Unknown
Public or Proprietary, Cost	Proprietary; the model is not publicly distributed outside ANL
Ease of use	Unknown
Ease of obtaining information and availability of technical support	The best point of contact is one of CASRAM's main developers, David F. Brown at ANL: <u>dbrown@anl.gov</u> (<u>https://www.anl.gov/profile/david-f-brown</u>).
Source code availability	No
Installation requirements/ software	Unknown
Maintenance Status	Still used as of mid-2020. The code is updated and maintained every 2-3 years, as per communication with David Brown.
Documentation	Information about the model can be found inside this 2017 technical document, although there is no official publicly available manual: https://www.phmsa.dot.gov/sites/phmsa.dot.gov/files/docs/training/hazmat/erg/7486/2016-erg-technical-document.pdf
Link to Website	See documentation above

8.8 CT-Analyst

Developer	U.S. Naval Research Laboratory
Type of Model	LES CFD Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Flexible for all types of CBRN releases within complex urban areas
Model Description	CT-Analyst is a hybrid plume dispersion model that provides an instantaneous, 3D, CFD LES model depiction of CBRN releases within complex urban areas to aid emergency responders in accidental or intentional airborne contaminant transport threats. The model simulates plume dispersion and propagation within the urban canopy at fine-scale resolution. Normally, LES simulations require lengthy processing and computational times, but CT-Analyst can produce dispersion results within seconds. Before a potential accidental release scenario, velocity fields are pre-computed for numerous meteorological conditions using NRL's high resolution LES transport model FAST3D-CT. The simulated database structure (called "dispersion nomografs") is processed into an efficient form used by CT-Analyst. It has also been shown to produce more detailed dispersion information with better results than more common Gaussian puff and plume models (Boris et al. 2003). The model was designed after 9/11 as a fast-response dispersion resource that can run with limited information about the source type. CT-Analyst can incorporate inputs from fixed and mobile sensors or inform the optimal locations for placing monitoring sites for model evaluation. The model uses principles of fluid dynamics and turbulence to simulate urban dispersion. Even though the steering wind direction and velocity magnitude influences the direction of plume spread, the specific urban morphologies and orientation of structures and streets control localized concentrations. Specifically, the model has high enough resolution to simulate building vortex shedding, recirculation zones, solar heating variations, and surface roughness
	(Boris et al. 2003). The model aims to better predict hazardous dispersion to avoid additional fatalities, exposures, and to plan the best course of evacuation.
Pros	through field studies and published conference proceedings
Cons	Preprocessing velocity fields is a lengthy process and may be difficult for responders; requires that FAST3D-CT be run for the specific case
Runtime	Simulation results are near-instantaneous and can be produced within seconds, but computational fields must be prepared ahead, which can take hours
Input Data Requirements	Measurements from isolated sensors (for model verification), general meteorological conditions (wind speed and direction)

Outputs	Dispersion plume that can be output to mapping services and rapidly disseminated
Data assembly requirements during or after emergency response	Limited information is needed, including a general sense of the release location, type, and local meteorology
Code language	Much of the source code and modules are written in Fortran
Public or Proprietary, Cost	The model can be downloaded by request at: <u>https://www.nrl.navy.mil/lcp/ct-analyst/download</u>
Ease of use	CT-Analyst has an easy-to-use interface that is simple to run once transport fields are generated through FAST3D-CT
Ease of obtaining information and availability of technical support	Questions or comments can be directed through the contact form at: <u>https://www.nrl.navy.mil/lcp/ct-analyst/contact</u>
Source code availability	No
Installation requirements/ software	Windows PC
Maintenance Status	Model is still used and supported by NRL
Documentation	See: Boris J.P., G. Patnaik, T. Young, Jr., 2003: CT-Analyst: Verification and Validation, NRL Report 4-1226-3377.
Link to Website	https://www.nrl.navy.mil/lcp/ct-analyst

8.9 **DEGADIS**

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Developer	University of Arkansas and the U.S. Environmental Protection Agency
Type of Model	Gaussian Plume Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Dense chemical gas releases over even terrain
Model Description	DEGADIS is a dense gas dispersion model used to simulate the concentrations of toxic chemical releases, especially for gases or aerosols heavier than the ambient air. The model can simulate evaporating pools and upward-directing or zero-momentum releases and jets, primarily over flat, level terrain. As one of EPA's alternative models, it can also predict the dispersion processes accompanying the gravity-driven flow and entrainment of the dense gas into the atmospheric boundary layer (Spicer and Havens 1989). DEGADIS is designed for zero-momentum, ground-level, area sources released from gas or aerosol clouds. The model can predict the downwind dispersion as a stably stratified plume or gas cloud. It has also been modified to simulate the vertical plume or cross section using the Pasquill-Gifford parameters to represent turbulent entrainment within the gas cloud. Although the model is primarily designed for ground-level sources, it can simulate the plume centerline and maximum concentration as a jet or plume lofts and then slumps back towards the surface due to gravity. The model can simulate continuous, finite (a constant rate over a short period of time), or transient (time-varying) release durations. DEGADIS, which is like the HGSYSTEM model in many ways, is freely available, evaluated, and recommended as an alternative model by EPA. DEGADIS has been tested and evaluated against some dense gas field and laboratory studies, although robust opportunities for these tests and evaluations are somewhat limited. Specifically, DEGADIS was evaluated using eight field over a short period opportunities for these tests and evaluations are somewhat limited. Specifically, DEGADIS was evaluated using eight field over a short period opportunities for these tests and evaluations are somewhat limited. Specifically, DEGADIS was evaluated using eight field over some sources and evaluated action are accent avaluation are somewhat limited. Specifically, DEGADIS was evaluated using eight field over some sources avaluated aconstruct
	experiments in Hanna et al. (1993) with a more recent evaluation against chlorine measurements from the JRII field study that is forthcoming.
Pros	Quick and accurate estimations of dense gas releases; model formulated on peer-reviewed dispersion principles (such as PGT stability classes, boundary layer similarity theories, and dense gas behavior); other models use DEGADIS formulations for their core dense gas dispersion
Cons	The free version of the model is run on a command line; otherwise, a paid GUI is available
Runtime	Fast
Input Data Requirements	General meteorological and boundary layer conditions; specifics about the release agent, duration, amount, and method

Outputs	Prediction of the downwind concentrations at various heights
Data assembly requirements during or after emergency response	General meteorological conditions; specifics about the release agent, duration, amount, and method
Code language	The source code is written in Fortran 77
Public or Proprietary, Cost	Available for free download through EPA's SCRAM website, or through the Breeze Software platform: <u>https://www.breeze-software.com/Software/LFG-Fire-Risk/Product-Tour/DEGADIS-Model/</u> . However, the Breeze GUI is not free
Ease of use	Moderate; runs from a Windows command line prompt. Versions using the GUI window make operation more straightforward
Ease of obtaining information and availability of technical support	Support for the EPA SCRAM website can be obtained by contacting George Bridgers: <u>bridgers.george@epa.gov</u> . Specific model support or questions can be directed to one of the developers, Dr. Tom Spicer: <u>tos@uark.edu</u>
Source code availability	Yes, on EPA's SCRAM website
Installation requirements/ software	Windows PC
Maintenance Status	Minor changes that do not change the model computations were introduced into DEGADIS v2.1 in September 2012
Documentation	A user's guide is available online at: https://www3.epa.gov/ttn/scram/userg/other/degadis2.pdf
Link to Website	https://www.epa.gov/scram/air-quality-dispersion-modeling-alternative- models#degadis

8.10 HotSpot

<u>HotSpot</u>

Developer	National Atmospheric Release Advisory Center (NARAC), Lawrence Livermore National Laboratory (LLNL)
Type of Model	Gaussian Plume Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Radiological releases in simple terrain regions
Model Description	HotSpot is a simplified Gaussian Plume model that provides emergency planners and responders a fast, field-portable set of software tools for evaluating radioactive release incidents. The model is designed for near- surface releases under short dispersion ranges and durations (less than 10 km and 24 hours). The model produces the best results under open terrain and simple meteorological conditions. Due to these limiting factors, HotSpot provides a fast but somewhat conservative means of approximating the effects of an accidental or intentional radioactive release. It can estimate continuous or instantaneous releases from explosions, fuel fires, and wide-area contamination events. The core dispersion model is built upon the general Gaussian Plume equation and accounts for various atmospheric stabilities, surface types and roughness, deposition, and plume rise (Homann and Aluzzi 2014). An additional tool estimates the effect of nuclear weapons, including neutron and gamma, blast, and thermal effects. The software also computes a first-order approximation of radiation and inhalation dose effects associated with explosions and facilities that handle nuclear materials. The model contains an extensive source term database and can simulate the dispersion of plutonium, uranium, tritium, and other radionuclides through plume, explosion, fire, and resuspension modeling methods.
	capabilities, and results can be exported to Google Earth or other GIS plotting software. The fast, yet conservative estimation of the radioactive release is designed so emergency responders can get a general sense of the episode (for example, ionizing radiation from the deposition of particles is ignored (Hill 2003)). Effective doses are estimated for the immediate and acute radiological impact on internal organs. The code also can estimate the potential fallout and arrival time, dose rate, and propagation of the fallout radioactivity after the release and as far as several weeks post-event.
Pros	Simple and fast, reasonable dose, exposure, and dispersion predication to inform emergency responders
Cons	Not for use during incidents with complex terrain or variable weather conditions; may underestimate some effects and provide a conservative prediction; susceptible to all limitations of Gaussian dispersion models

Runtime	Fast, 15-30 seconds or less
Input Data Requirements	Isotope release type, mass, and general meteorological conditions
Outputs	Hazard zones and dose estimates from release plume
Data assembly requirements during or after emergency response	Information about the release type and amount, general weather conditions
Code language	Visual Basic, Microsoft .NET Framework
Public or Proprietary, Cost	The latest version can be freely downloaded by filling out by registering as a HotSpot user at: <u>https://naracweb.llnl.gov/web/hotspot/registerUser.html</u> without having to have a NARAC account.
Ease of use	Very easy for most users, simplified GUI
Ease of obtaining information and availability of technical support	While a public help forum does not exist, questions or problems can be directed to <u>hotspot@llnl.gov</u>
Source code availability	No
Installation requirements/ software	Windows PC
Maintenance Status	Currently operated and updated by LLNL to incorporate the most current radiological dose conversion methodologies; Current Version 3.1.2 as of mid-2020
Documentation	The user's manual can be downloaded at: https://narac.llnl.gov/content/assets/docs/HotSpot-UserGuide-3-0.pdf
Link to Website	https://narac.llnl.gov/hotspot

8.11 HPAC

Developer	U.S. Department of Defense (DOD), Defense Threat Reduction Agency (DTRA), and Applied Research Associates, Inc. (ARA)
Type of Model	Gaussian Puff Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Various CBRN releases in complex terrain and urban areas
	The HPAC model is a comprehensive, operational, and research-grade CBRN dispersion modeling system that integrates high resolution meteorological data (DTRA 2004). It can be used for hazardous release-agent planning purposes (i.e., "forward deployable") or through reach back service for civilian and military populations. The model can be applied to a wide variety of defense, industrial, or transportation-related accidents. HPAC is the primary model used by DTRA for IMAAC emergency response plumes and can typically be delivered to customers within 20-30 minutes after the initial request. The model can be activated quickly because DTRA automatically pulls in real-time NWS weather data and archives it on their meteorological data servers. These databases also store worldwide NWP products and climate reanalysis data. Historical weather for numerous locations can also be accessed. The model has been in use since 1995 and is managed by DTRA out of Ft. Belvoir, VA. HPAC is used extensively with the DOD and has been evaluated for several urban field experiments (Chang et al. 2005), and most recently by Miner et al. (2019).
Model Description	HPAC's primary transport and dispersion model is built up on the SCIPUFF Gaussian puff model (Sykes et al. 2007) that has been extensively tested and developed since the 1980s. SCIPUFF, which has also been incorporated within many other dispersion models, permits fast computational times (within minutes) and many advanced capabilities, including atmospheric transport and dispersion plume estimations, urban parameterizations, deposition, dose, and human effects-hazards. The source term can be identified by a particle size distribution and can incorporate continuous, instantaneous, and finite duration releases. NCAR's Hazardous Material Source Term Estimation tool ⁵ is also being used and developed within HPAC to streamline the input process. SCIPUFF uses the detailed NWS meteorology to simulate time and space- varying puffs from the effluent source that travel downwind and disperse, resulting in an accurate representation of the atmosphere at the time and location of the release, including splitting puffs when they grow too large due to wind shear and turbulence (Miner et al. 2019). Recent additions to SCIPUFF simulate the effects of potential radioactive releases from nuclear weapons or power plant reactor accidents and modifications for dense gas and simple chemistry and aerosols. HPAC/SCIPUFF also uses urban canopy modifications to account for changes in the wind speed profile (Cionco 1978)

Hazard Prediction Assessment Capability (HPAC) Model

⁵Visit this link for more information: <u>https://nar.ucar.edu/2018/ral/hazardous-material-source-term-estimation</u>

	as well as urban parameterizations from DSTL's UDM (Hall et al. 2002). While UDM does not resolve dispersion around individual buildings, it modifies a plume based on street alignment and building density in urban areas. SCIPUFF can also account for variations in the terrain and land surfaces, which tends to have a large influence on the plume transport. Digital terrain elevation files are used to develop mass consistent wind and turbulence within the model through natural obstacles. Many additional capabilities are also built into HPAC, all of which is run through a GUI window.
Pros	Fast access to real-time weather data through meteorological data servers; extensively evaluated with field data and shown to have good performance; used operationally by many government entities
Cons	May be complicated to use without knowledge of the software; not a large online support base (but HPAC instructional classes exist)
Runtime	Moderately fast (within 15-30 minutes or less)
Input Data Requirements	Time and location of the release, information about the source term
Outputs	Dispersion plume with estimated hazard zones downwind of the source
Data assembly requirements during or after emergency response	Time and location of the release, information about the source term; HPAC is also used when resources are requested through IMAAC.
Code language	The core SCIPUFF code is written in FORTRAN 90 but operation of HPAC is streamlined through a GUI window
Public or Proprietary, Cost	Available for free to US Government employees and contractors, other government-related uses, and to academia by emailing the software distribution officer: <u>Bonnie.a.cassano.ctr@mail.mil</u> or the first email address under the technical support box below. An application is required and will be submitted to DTRA for approval.
Ease of use	Moderate, due to input options
Ease of obtaining information and availability of technical support	User support and assistance can be obtained by emailing: <u>dtra.belvoir.rd.mbx.Reachback-Software-Distribution@mail.mil</u> . Help regarding the meteorological data server and archived weather can be directed to: <u>dtra.belvoir.rd.list.meteorological-data-services@mail.mil</u>
Source code availability	No
Installation requirements/ software	Windows PC with at least 20-25 GB of free hard drive space if the entire archived meteorological data is desired

Maintenance Status	Continuously updated and improved by DTRA and its contractor ARA. A recent stable release was HPAC v6.5 (mid-2018)
Documentation	The HPAC v4.04 user's guide available in PDF at: <u>ftp://ftp.atdd.noaa.gov/pub/gunter/hpac_404_users_manual.pdf</u> for online viewing; the newest HPAC model releases include the documentation within the root directory on the CD shipped from DTRA
Link to Website	HPAC is currently (as of mid-2020) not posted on DTRA's Research and development website: <u>https://www.dtra.mil/Mission/Mission-</u> <u>Directorates/Research-and-Development/</u> but information about the model can be obtained through <u>https://www.acq.osd.mil/ncbdp/nm/narp/Radiation_Data/Specialized_Radiolo</u> <u>gical.htm</u> and the following papers: Miner et al. (2019), Chang et al. (2005), and several others.

8.12 HYSPLIT

Developer	NOAA Air Resources Laboratory (ARL)
Type of Model	Lagrangian Stochastic Particle Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Local-to-regional forward and backward trajectory of particles or air parcels
Model Description	HYSPLIT is NOAA's Lagrangian dispersion model that calculates simple forward and backward air parcel trajectories, contaminant transport, chemical transformation, and deposition of particles, gases, or aerosols over regional (mesoscale) or long-ranges (synoptic; >1000 miles) (Stein et al. 2015). Due to its high fidelity of operation, it is one of the most used transport and dispersion models in the world. The model can generate trajectories using archived, gridded meteorological model data for past episodes or gridded model simulations for future predictions (Draxler et al. 2020). HYSPLIT can be run rather quickly through an internet browser on NOAA's ARL READY website for archived episodes, or through reanalysis data from as far back as 1949. Additionally, it can be downloaded and run locally on a Windows PC, Mac, or LINUX workstation through a GUI or script. The latter is used mainly for research purposes and can be driven with weather forecast data generated from models like WRF. There are at least 15 options for gridded 3D meteorology inputs using global or North American datasets. The gridded wind fields on the READY website contain horizontal resolutions ranging from 3 km to 1° and various vertical resolutions using pressure- and elevation-related coordinate systems. Many users run a backward trajectory analysis at a receptor site to determine the origin of an air mass or contaminant source. The model can calculate the dispersion of an unknown material point source (instantaneous or long duration), where it calculates the forward trajectory of generic particles. It can also simulate prescribed burns, wildfire smoke, and volcanic eruptions. HYSPLIT calculates the advection and diffusion using a Lagrangian moving frame of reference as the trajectory of particles or parcels move from their original location. The model simulates transport interactions at and between multiple levels above the earth's surface. Pollutant dispersion is calculated through a series of puffs as they advect downwind. Many options suc
Pros	Fast, free, and well-documented with large support base; model has been extensively evaluated and used in the atmospheric sciences field and is used

Hybrid Single Particle Lagrangian Integrated Trajectory Model (HYSPLIT)

	operationally within NOAA; provides an accurate representation of plume due to time-varying and high-resolution meteorology
Cons	May not provide as much detail on local dispersion-related effects as some emergency responders require; needs complex gridded wind input datasets
Runtime	Fast (seconds through the READY website platform)
Input Data Requirements	3D gridded meteorological model data, basic information about release source
Outputs	Dispersion plume or (forward or backward) spatial trajectory of source or receptor, which can be plotted or output to Google Earth
Data assembly requirements during or after emergency response	Meteorological model data from the most recent NOAA model runs (i.e., NAM, GFS, or HRRR) can be gathered through the READY website; basic information about release source
Code language	Most of the source code is written in Fortran
Public or Proprietary, Cost	Freely available through NOAA ARL's website
Ease of use	Web-based use is very simple, and results can be generated within minutes with limited prior use. Other versions (i.e., through the LINUX command line and using forecast model data) may be more complicated for some users
Ease of obtaining information and availability of technical support	A large support forum to communicate questions, improvements, problems, and ideas is available through: <u>https://hysplitbbs.arl.noaa.gov/</u> . Various technical tutorials are also available for self-paced training: <u>https://www.ready.noaa.gov/HYSPLIT_Tutorials.php</u>
Source code availability	Source code repository is available for non-commercial use only to a limited number of registered users. Interested parties can send a request via email to <u>arl.webmaster@noaa.gov</u> , but granting the request is subject to the discretion of HYSPLIT developers. Modifications or improvements to the source code are expected to be shared with the HYPLIT user community
Installation requirements/ software	Model can be run through a browser, or locally on a 64-Bit Windows PC, Mac, or through the command line on LINUX systems. Users do not need to register to use the web-based trajectory or dispersion software using archived meteorological data. Registration is only required to use forecast data or to download the LINUX or registered versions for PC or Mac computers. Registration is permitted for government, commercial, educational/academia, or non-profit users.
Maintenance Status	Continuously updated and improved. The most recent version as of mid-2020 is HYSPLIT v5.0.0 released in April 2020. Status updates are posted on: https://www.arl.noaa.gov/hysplit/hysplit-model-updates/
Documentation	A complete web-based user's guide is available at: <u>https://www.ready.noaa.gov/hysplitusersguide/</u> or through NOAA Technical Memo ERL-ARL 230 (Draxler 1999) along with other self-paced resources
Link to Website	https://www.ready.noaa.gov/HYSPLIT.php

8.13 JEM

Joint Effects Model (JEM)

Developer	Department of Defense (DOD); Aeris, LLC.
Type of Model	Gaussian Puff Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	For most CBRNe releases in remote or urban areas
Model Description	JEM is a comprehensive and operational dispersion modeling software application used to simulate accidental or intentional CBRNe incidents and weapon strikes. The model is widely used within the U.S. military with advanced capacities for complex terrain, TICs, human health indications, and urban environments. The model is browser-based and runs through an internet application to allow for portable and near real-time simulations following various types of releases or strikes, although it can also be run on a stand-alone system. JEM is primarily supported, maintained, and used by the US Army and DOD. It is currently the only accredited tool to effectively model impacts from hazardous releases by assisting warfighters in planning for and mitigating the effects of WMD. The model simulates the impact of downwind dispersion based on various weather conditions (wind speed, direction, and atmospheric stability), terrain, local structures, and release material interactions. The DOD can generate JEM results on a 24/7 basis through its internet and telephone reach back service. JEM can also be implemented for strategic or tactical use within the U.S. or overseas. JEM's core dispersion model is built upon the SCIPUFF Gaussian Puff Model (Sykes et al. 2007) to simulate time and space-varying puffs from the effluent source that travel downwind and disperse. This is the same model that drives the dispersion component in HPAC. For more information about SCIPUFF, see the entry for HPAC in Section 8.11 . JEM contains two options for urban dispersion: an urban canopy parameterization based on wind and turbulence profiles from SCIPUFF, and the UDM model from DSTL (Hall et al. 2004). UDM was also provided in the quick reference table. A comprehensive evaluation of JEM from four different urban field studies has been reported in Chang and Hanna (2010) and Hanna and Chang (2012). JEM versions 1 and 2 are currently in use, although JEM 1 is being phased out to support more modern computer technologies. JEM replaces and/or incorporate
Pros	The only DOD-accredited tool to simulate CBRNe dispersion for warfighting and tactical purposes; uses well-documented and evaluated SCIPUFF model framework
Cons	Mainly for military use, although some external research use is possible
Runtime	Fast

Input Data Requirements	Wind direction and speed, release specifics
Outputs	Spatial estimation of plume from release
Data assembly requirements during or after emergency response	Meteorology (wind speed, wind direction, and a general indication of weather conditions and atmospheric stability) near the release location, method and type of release and rate of emission
Code language	The core of SCIPUFF is written in FORTRAN 90 but operation of JEM is streamlined through a GUI for most uses
Public or Proprietary, Cost	Mainly for use by DOD, contractors, and some foreign militaries (e.g., Spain and Canada)
Ease of use	Web-based GUI simplifies operation
Ease of obtaining information and availability of technical support	Not known
Source code availability	No
Installation requirements/ software	Windows PC-based; also deployed on UNIX systems and is integrated into Command and Control C2 systems across the DOD. The model is available in a stand-alone version or through a networked or web platform
Maintenance Status	The latest version is JEM 2 as of mid-2020 with planned continual development, integration, and deployment, and additional cloud-based capabilities to at least FY23. JEM 2 is still being evaluated and improved with field study data
Documentation	A comprehensive technical document for the JEM model does not exist (Hanna and Chang 2012). The transport and dispersion model specifics can be found in the SCIPUFF documentation by starting at: <u>http://www.scipuff.org/</u>
Link to Website	https://asc.army.mil/web/portfolio-item/joint-effects-model-jem/

8.14 MELCOR and MACCS

Developer	Sandia National Laboratory (SNL)
Type of Model	Gaussian Plume Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Around and adjacent to nuclear power plant sites; radiological/nuclear releases
Model Description	MACCS is a comprehensive straight-line Gaussian plume model package used to develop a probabilistic risk assessment from a severe accidental atmospheric release of radioactive material from light water nuclear power plants (Chanin et al. 1998). Mainly developed and used for and by the NRC since 1990, MACCS simulates ecosystem and human dose and exposure impacts within and adjacent to nuclear power plants. It can diagnose potential land contamination levels, exposure and risk to susceptible populations based on recommended response actions and economic losses resulting from an accident. MACCS incorporates wind and atmospheric turbulence from time- varying meteorology, plume rise, wet and dry deposition, inhalation, cloud and ground shine, ingestion, and shielding. The suite of codes contains MelMACCS (the preprocessor code that interfaces MELCOR, the process analysis code simulating the chain of events during a meltdown, with MACCS), WinMACCS (a graphical user interface), SecPop (a program to generate consequence calculations based on population, land use, and economic databases), and COMIDA2 (a food pathway model to estimate doses of radionuclides from consumption). MACCS provides a comparative assessment of various dose-threshold models to more objectively quantify the uncertainty of various inputs. The model also incorporates a road network model to suggest the best evacuation routes to limit exposure from the radioactive release and corresponding plume.
	MACCS is used to inform emergency preparation and response guidance around reactor sites. The NRC requires all nuclear power plants applying for or renewing operating licenses to perform cost-benefit analyses using MACCS. The software suite is currently the only code used by the NRC to inform Level 3 critical nuclear episode risk assessments post-release. Additionally, the DOE uses MACCS to assess safety by demonstrating emissions at powerplant boundaries remain below regulatory limits. The NRC may also use MACCS for modeling and risk analysis support for IMAAC. Recent uncertainty analyses called the State-of-the-Art Reactor Consequence Analyses (SOARCA) project have documented best modeling practices from numerous studies and current knowledge on severe nuclear accidents (Chang et al. 2012). SNL also provided severe accident modeling support during the Fukushima Power Plant disaster.
Pros	No other U.S. publicly available dispersion modeling and consequence analysis code currently offers all MACCS's capabilities; currently supported by the NRC for risk analyses, planning, and power plant licensing; continuously enhanced and improved

MELCOR Accident Consequence Code System (MACCS)

Cons	Mainly used by staff at DOE facilities; model is susceptible to all inherent limitations and simplifying principles of Gaussian plume models; MELCOR is complex to use if the user is not familiar with power plant controls
Runtime	Model runs rapidly (within seconds to minutes) once configured
Input Data Requirements	Local meteorology, nuclear powerplant information. WinMACCS contains databases of local populations, economic situations, and land use.
Outputs	Series of risk and consequence analyses
Data assembly requirements during or after emergency response	Local, time-varying meteorology (wind speed, wind direction, and a general indication of weather conditions), method of accident and potential rate of emission
Code language	FORTRAN
Public or Proprietary, Cost	Public distribution to domestic utilities, vendors, academic institutions, commercial enterprises, and some international organizations by filling out a non-disclosure agreement. The software is free to academic institutions, NRC contractors, U.S. federal government, and some international government organizations although no technical assistance is provided. There is a \$2,500 one-time fee for shipping, handling, and installation service for commercial organizations only.
Ease of use	Running, setting up, and producing the output from MELCOR is potentially time-consuming. However, a program called MelMACCS has been developed to streamline the source integration and the dispersion component to the consequence analysis software, which acts as a preprocessor interface.
Ease of obtaining information and availability of technical support	No technical assistance is provided, but certain program assistance and questions can be provided through <u>wg-maccs-entity@sandia.gov</u> or for a fee.
Source code availability	No
Installation requirements/ software	The software runs through an application call WinMACCS 4.0, a graphical user interface that streamlines model setup and results
Maintenance Status	The latest version of MACCS is 4.0 as of mid-2020. The software is currently implemented across DOE platforms with continuous maintenance for current and future reactor designs. Code modernization is underway. The MACCS Development Team is working to couple the model with HYSPLIT as an alternate and improved dispersion model. Additional features to evaluate economic impacts on gross domestic product from power plant accidents is also underway.

Documentation	An extensive description of the MACCS dispersion model is available at: <u>https://maccs.sandia.gov/docs/MACCS_factsheets/MACCS%20Model%20De</u> <u>scription.pdf</u> .
	MACCS User's guide: <u>https://maccs.sandia.gov/docs/MACCS_factsheets/Code%20Manual%20for%</u> <u>20MACCS2%20Vol%201.pdf</u>
	MELCOR also has its own set of code manuals: https://www.nrc.gov/docs/ML1704/ML17040A429.pdf
Link to Website	https://maccs.sandia.gov/maccs.aspx

8.15 QUIC

Developer	Los Alamos National Laboratory (LANL), DOE (PI: Michael Brown)
Type of Model	Lagrangian particle, random walk urban dispersion model
Response Stage	Emergency Preparedness
Original Application	Various CBRNe releases within urban areas
Model Description	QUIC is a relatively fast Lagrangian dispersion model that can compute pollutant dispersal on the building-to-neighborhood scale (Nelson and Brown 2013). It is "CFD-like" in the sense that it simulates detailed wind flow and pressure fields around obstacles but runs relatively quickly on a laptop depending on the domain size and release specifications. The model contains algorithms that calculate flow fields around building profiles and through street canyons (Brown 2014) based on the work of Röckle (1990), with improvements from Nelson et al. (2008, 2009) and others. The addition of buildings could produce more realistic results around obstacles and through street intersections since certain neighborhoods could receive higher pollutant concentrations while others remain relatively unaffected due to building wake and cavity effects. When setting up the QUIC simulation through its GUI, a shapefile can be imported with building dimensions, or the user can develop their own domain using <i>CityBuilder</i> . The model can be run using an inner and outer domain to expedite the simulation and to develop the appropriate turbulence fields as the wind encounters the inner focus area. QUIC includes a 3D wind field model called QUIC-URB that generates the flow conditions around the urban obstacles. The local meteorology (wind speed and direction) is added via the <i>MetGenerator</i> tool. A module calculates the vertical wind profile based on theoretical boundary layer scaling equations, or the user can import their own profile. Various wind profiles can also be implemented within the domain as a function of time. The placement and specification of the calculates concentration and deposition fields from the flow generated in QUIC-URB. QUIC can account for a variety of point, area, and line CBNNe releases with more advanced properties, including dense gas, evaporation, and buoyant dispersion effects. Custom properties related to the release type such as specifications of a toxic gas or particle size distribution, amount, location, an

Pros	Relatively fast running and accounts for building and street canyon effects in a realistic way; evaluated against field and laboratory data (Brown et al. 2013), many flexible input options
Cons	The learning curve can be high depending on application; lack of model support, lack of output formats for postprocessing
Runtime	Seconds to < 1 hour
Input Data Requirements	Buildings must be in shapefile format or constructed within QUIC-GUI, accurate details about source terms and meteorology
Outputs	2D and 3D spatial plots of contaminant deposition or concentration
Data assembly requirements during or after emergency response	Moderate-high due to complex source term classifications
Code language	FORTRAN in executables, run through MATLAB
Public or Proprietary, Cost	Free for researchers, government employees, contractors, and academia
Ease of use	Moderate; requires user to be familiar with user's manual, but run through GUI window
Ease of obtaining information and availability of technical support	No formal user support group but users can email developer for questions or assistance: <u>mbrown@lanl.gov</u>
Source code availability	No, unless working with developer to improve model
Installation requirements/ software	None; works within MATLAB, but an executable is provided to run the model as a standalone version. Runs on 32- and 64-bit Windows and Mac computers.
Maintenance Status	Continuously improved, currently v6.26 in 2018
Documentation	Well documented user's manual: https://www.lanl.gov/projects/quic/open_files/QUICv6.01_StartGuide.pdf Several peer reviewed publications and conference proceedings.
Link to Website	https://www.lanl.gov/projects/quic/

8.16 SHARC/ERAD

Specialized Hazard Assessment Respon	se Capability/Explosive Release Atmospheric
Dispersion (SHARC/ERAD)	

Developer	Sandia National Laboratory (SNL)
Type of Model	Gaussian Puff Dispersion Model
Response Stage	Both Emergency Preparedness and Response
Original Application	Radiological dispersal devices (RDDs), radiological/nuclear and explosive release types over flat terrain
Model Description	SHARC/ERAD is a suite of five models that simulates the release of radioactivity from nuclear weapon explosions, RDDs, or other accidental or intentional detonations. The software assesses the time-dependent dynamic explosive buoyant plume rise and then estimates the associated human exposure and evacuation decisions through an integrated geographic information system and population databases. The SHARC model package contains Nuke 2.0 to predict the immediate nuclear and radiation effects, AIRRAD 2.0 for nuclear fallout estimations, Blast 2.0 to provide effects from the explosion, ERAD 7.0 for the dispersal of radioactivity by explosively driven plume rise or through conventional non-buoyant releases, and MCK, which is the Monte Carlo Gaussian puff model for plume dispersion ⁶ . The 3D puff dispersion model was first developed in the 1980's to assess the time- dependent buoyant rise and atmospheric transport for different meteorological conditions. It incorporates various surface roughness lengths for even terrain types and models vertical diffusion using a Monte Carlo method, a random and probabilistic approach adapted for turbulent dispersion. SHARC can simulate multiple scenarios based on the time and location of the event. It can predict nuclear fallout patterns and provide guidance for short- term relocations and long-term evacuations. Fatalities, casualties, and exposure estimates are determined though U.S. Census and Landscan data with the ability to export graphical products to Google Earth or other GIS platforms. The software produces automated graphical displays of areas affected by the radiation and can develop integrated reports on the incident for responders. With advance notice of a nuclear or RDD threat, SHARC contains a decision support tool to determine the best way to move the device out of the area. In addition, SHARC is incorporated within the Turbo FRMAC (Federal Radiological Monitoring and Assessment Center) software to calculate official federal response guidance and inform the proper act
Pros	Moderate input data requirements, vertical variation in meteorology, fast computational time (which allows for multiple scenarios to be run), population databases for a wide variety of locations

⁶ For more information, see: <u>https://www.osti.gov/servlets/purl/1124469</u>

Cons	Able to simulate only under flat and open terrain, software restricted to explosive and RDD releases
Runtime	Fast, approximately 2-5 minutes execution time
Input Data Requirements	1-D vertical wind and temperature profiles for a single time period
Outputs	Fallout pattern, casualties, sheltering, evacuation guides, containment and mitigation effects
Data assembly requirements during or after emergency response	Local 1D meteorology, source term and knowledge of the release
Code language	Not known
Public or Proprietary, Cost	Available to the international emergency response community upon request through SNL's Nuclear Incident Response Program at: <u>https://nirp.sandia.gov</u>
Ease of use	GUI simplifies operation
Ease of obtaining information and availability of technical support	Questions can be directed to: <u>nirp-support@sandia.gov</u> or <u>nirp-</u> <u>fogbugz@sandia.gov</u> regarding specific inquiries about the software
Source code availability	No
Installation requirements/ software	Windows PC or Workstation; runs through GUI and combined with SNL's Turbo FRMAC
Maintenance Status	Continuously maintained; current version is SHARC 2019 ERAD v7.0 as of mid-2020
Documentation	User's manual available once software and account are requested and created on SNL's website
Link to Website	https://nirp.sandia.gov/Software/SHARC/

9.0 Concluding Remarks

Atmospheric dispersion models have evolved substantially since their introduction into the emergency response community. The foundations of atmospheric transport and dispersion theory were developed almost 100 years ago, but simple dispersion models that calculate downwind plume concentrations were not introduced until the 1960s. These models, developed extensively over the following decades, were used mainly to assess pollution levels from point emission sources, such as single effluent stacks and industrial sites. The terrorism on US soil in 2001, and subsequent fear post-9/11 encouraged the growth and improvement of higher fidelity dispersion models, especially for urban areas with greater threats for human exposure. Other homeland security threats, such as powerplant accidents, biological releases, or chemical spills also demonstrate the critical need for dispersion modeling to be continuously tested, developed, and improved. Dispersion modeling offers a crucial insight for emergency preparation or planning scenarios so responders can be well-equipped and make knowledgeable decisions. Dispersion modeling has also proved to be a critical component during the emergency response (Leitl et al. 2016) and post-response stages to inform evacuation of affected communities, sample for contamination, decontaminate surfaces, and manage waste generated from the recovery process.

The goal of this report is to briefly explain the fundamental concepts of atmospheric transport and dispersion and provide a comprehensive database of dispersion models that can be used for emergency preparation and response to facilitate discussion between public, private, academic, and/or government sectors that use them. The abundance of model options often creates confusion and results in challenging decisions on the type of model to use for a specific scenario. A comprehensive model review of this magnitude has not recently occurred. This report also provides background information and a literature review on previous model review efforts. Much of those databases laid the foundation for this work, with modifications and additions for the current state of dispersion modeling. The report also provides introductory concepts on boundary layer meteorology and the various types of dispersion models. A basic understanding of the physical processes governing how dispersion models work is crucial when interpreting the results. This work is intended to provide a quick reference for those new to dispersion modeling or for those seeking to expand their knowledge base. It is not meant to replace primary literature sources such as textbooks.

This report outlines and alphabetically sorts dispersion models with potential applications for CBRNe risks. An extensive quick reference table for 96 different dispersion models is provided in **Section 7.0.** Sixteen of those models were selected for a more detailed, two-page review in **Section 8.0** due to their potential applicability and usefulness for emergency response. Twenty-four models were also identified that could be potentially useful, but additional research is needed by the user to decide if that model is a viable fit. The model review was not meant to recommend or endorse a specific model but to provide users with a resource of options that document the currently available models so they can make their own informed decisions. Additionally, this resource is not meant to take the place of other Federal dispersion modeling options and reach back services such as IMAAC and NARAC.

Similar to the results presented in Mikelonis et al. (2018) and EPA (2018), no one single model is found to have all the requirements conceived as beneficial during consequence management of a wide area response. Out of the 16 dispersion models selected for detailed analysis, six were Gaussian Plume models, four were Gaussian Puff models, four were Lagrangian particle models, and two were CFD or LES model. A few models incorporated both Gaussian Puff and Plume relationships. The model review results in the following observations:

1) Most dispersion models are developed and maintained by Federal government agencies or National Laboratories
- 2) Most CBRNe models are not widely distributed to the public and require certain criteria to obtain the model, such as being a government employee, contractor, or within academia
- 3) Most emergency response models are Gaussian plume or puff models that run quickly, while emergency preparation models are Lagrangian or CDF-based
- 4) Model runtime is usually related to the model's complexity
- 5) Finding model support may be difficult for many models, and some are not widely described or documented online
- 6) Model complexity depends mainly on the user's expertise, available hardware, the overarching model framework, and the input data requirements
- 7) Input data, especially to the detail most models require, may not be available immediately postrelease. This is a crucial time when the model is needed for emergency response guidance.
- 8) A quantification of model uncertainty is usually not depicted directly by the model, but may be accomplished by rerunning the model with different input options or tuning the parameters
- 9) Most dispersion models are built upon the same underlying framework and mathematical equations based on fundamental dispersion and turbulence theories
- 10) There is extensive overlap in the capabilities of dispersion models, with additional elements built for specific purposes related to the agency's mission
- 11) Many models are site-specific or research grade
- 12) Source codes are generally not released by the developers
- 13) More user-friendly and mobile model options are needed, particularly with intuitive user interfaces though laptops, smartphone apps, or through remote cloud-computing.

Based on the review presented here, an acceptable balance of speed, model performance, ease of use, and purpose of application should clearly be established when choosing a dispersion model. The review shows that complex Lagrangian or CFD models have greater data requirements and runtimes that may not be readily available in an emergency scenario. As noted by Mikelonis et al. (2018), the choice of modeling software may also be influenced by existing software and personnel expertise in an affected location. Among EPA-developed models, users have a variety of choices in dispersion models since many have been developed for research or regulatory use. Most of the model codes are open source and easily obtainable. User support and troubleshooting is available, and models are well documented. As a result, EPA's AERMOD dispersion model is a viable option to consider for future development for contaminant fate and transport following a hazardous release event because of the availability of the source code and robust model framework that has been extensively designed by, and evaluated with, field and laboratory data. In particular, AERMOD could benefit from additional beta (test) options to better account for wind profiles influenced by buildings and street canyons. Urban modifications or parameterizations may be some of the most important developments for future versions of dispersion models used in emergency preparation and response.

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